



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
CENTER FOR ENVIRONMENTAL MEASUREMENT AND MODELING  
RESEARCH TRIANGLE PARK, NC 27711

OFFICE OF  
RESEARCH AND DEVELOPMENT

February 23, 2022

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NJ Department of Environmental Protection  
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**Subject:** NJ DEP Data Report #11: Non-targeted Analysis of PFAS in Wastewater and Groundwater Samples Collected at the Solvay Specialty Polymers Plant in West Deptford, N.J.

Dear Mr. Kloo:

I am pleased to provide you with the attached laboratory report that includes non-targeted analysis (NTA) results for per- and polyfluoroalkyl substance (PFAS) in water samples collected from wastewater and groundwater influent associated with the Solvay Specialty Polymers plant in West Deptford, NJ. This is the eleventh in a series of reports prepared as a part of EPA Office of Research and Development's (ORD) collaboration with the New Jersey Department of Environmental Protection (NJ DEP) and EPA Region 2 on the study, "Detection, Evaluation, and Assignment of Multiple Poly- and Perfluoroalkyl Substances (PFAS) in Environmental Media from an Industrialized Area of New Jersey."

It is our understanding that this study was designed to help NJ DEP in their ongoing investigation into the presence of PFAS in the environment near manufacturing facilities of interest. This study relates to our research capabilities and interests applying targeted and non-targeted analysis methods for discovery of the nature and extent of PFAS environmental occurrence that may be potentially associated with industrial releases. EPA continues to develop analytical methods for many PFAS compounds in various media including some of those included in this report. We are providing the results of our analysis as they become available.

In this report, we provide tentative identification and semi-quantitative analytical results for PFAS compounds. We do not interpret exposure or risk from any reported values. EPA does not currently have health-based standards, toxicity factors, or associated risk levels for PFAS, other than perfluorooctanoic acid (PFOA), perfluorooctane sulfonate (PFOS), perfluorobutanesulfonic acid (PFBS), and GenX chemicals. While the data provided in the attached report indicate the presence of PFAS in the water samples, we do not have sufficient information to offer interpretations related to human or environmental exposure and risk.

Thank you for inviting us to be part of this effort that helps to further both EPA's and New Jersey's understanding of an important issue in the state. This is just one of many Agency efforts that demonstrates EPA's commitment to cooperative federalism.

If you have any questions or concerns, do not hesitate to contact me at (513) 569-7852 or via email at [gilliland.alice@epa.gov](mailto:gilliland.alice@epa.gov). I look forward to our continued work together.

Sincerely,

A handwritten signature in cursive script, appearing to read "Alice Gilliland".

Alice Gilliland

Director, Acting

Enclosure

CC:

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## **Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey**

### **Laboratory Data Report #11: Non-targeted Analysis of PFAS in Wastewater and Groundwater Samples Collected at the Solvay Specialty Polymers Plant in West Deptford, N.J.**

**Background.** This report stems from a collaborative study with EPA ORD, EPA Region 2, and NJ DEP entitled “Detection, Evaluation, and Assignment of Multiple Poly- and Perfluoroalkyl Substances (PFAS) in Environmental Media from an Industrialized Area of New Jersey.” NJ DEP assumed responsibility for the collection of samples and their shipment to the ORD laboratory. ORD was responsible for sample extraction and analysis of PFAS. Preparation of this report involved many from ORD assuming various roles and responsibilities (Table 1).

**Table 1. EPA Office of Research and Development Lab Analysis and Report Team.**

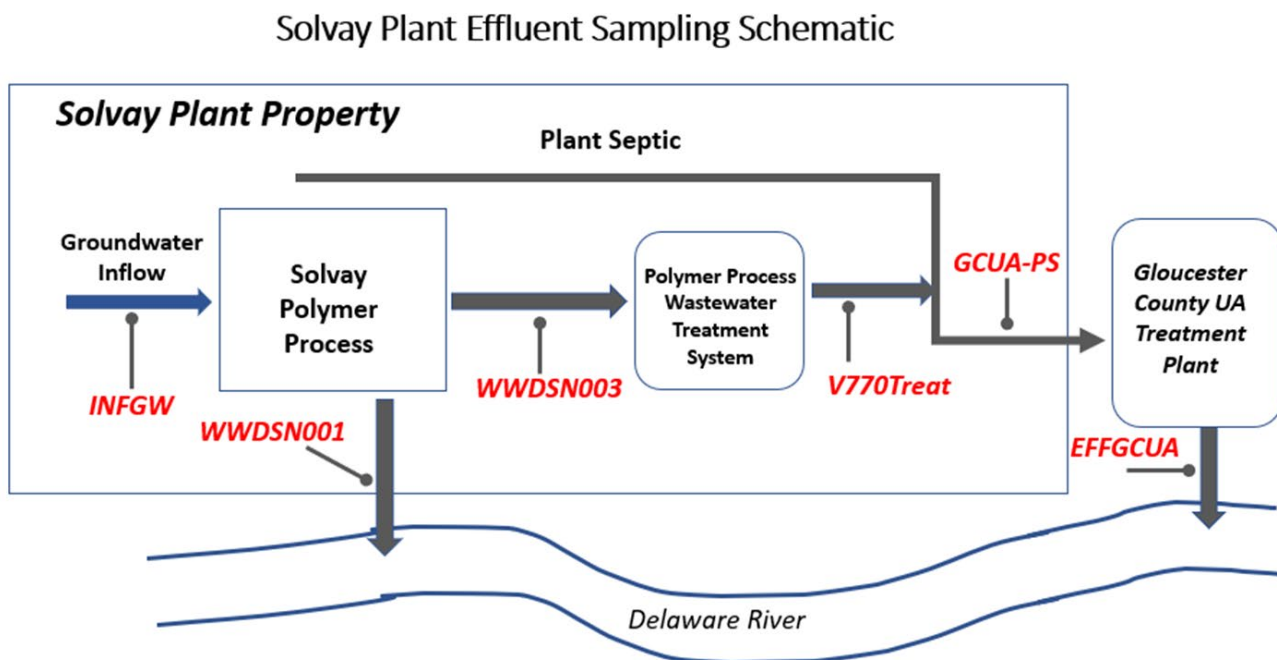
<b>Responsibility</b>	<b>Personnel</b>
ORD Principal Investigators	James McCord, Mark Strynar, John Washington
Laboratory chemistry	James McCord
Quality Assurance Review	Margie Vazquez
Management coordination and review	Kate Sullivan, Myriam Medina-Vera, Brian Schumacher
Report preparation	Kate Sullivan, James McCord

This 11<sup>th</sup> report includes results of non-targeted analysis for PFAS in 13 water samples collected by NJ DEP from wastewater and groundwater influent locations at the Solvay Specialty Polymers (Solvay) plant and from the Gloucester County Utility Authority (GCUA) located in West Deptford. GCUA receives Solvay wastewater after post-process treatment. Samples were collected on March 10, 2021 with repeated sampling on April 6, 2021 when a different manufacturing process was operative.

The samples were collected from water inflow and wastewater effluent at 6 locations in the Solvay Plant or following treatment at the Gloucester County Utility Authority (GCUA) as shown in Figure 1. To evaluate the potential for PFAS to be present in Solvay’s process source water, groundwater influent was collected prior to the treatment or fluorochemical processes as represented by INFGW. Effluent from the polymer process is discharged either directly to surface water from the permitted NJPDES outfall represented at location WWDSN001, or it is sent to the polymer process wastewater treatment system within the Solvay Plant. The polymer process effluent is sampled pre-treatment as represented by WWDSN003. After treatment, the effluent is comingled with the plant septic system before it is sent to the GCUA for final treatment. Due to these concerns raised by NJ DEP during its sampling on March 10, Solvay installed a sampling port on the pump that directly discharges industrial wastewater from the polymer process

wastewater treatment system (V770-TREAT). According to Solvay, water at this sampling port eliminates any sanitary discharge interference and best represents the treated effluent from the polymer process as it exists prior to discharge to the GCUA. The co-mingled effluent from the polymer treatment and plant septic is sampled at GCUA-PS before it enters GCUA for final treatment. GCUA discharges treated effluent to the Delaware River as represented by sample EFFGCUA.

**Figure 1. Schematic for wastewater effluent sampling locations at the Solvay plant in West Deptford. The approximate location of sample with naming conventions are in red lettering.**



Samples collected March 10 were delivered to the ORD laboratory in Research Triangle Park, NC on March 11, 2021 and the second set of samples was delivered April 7, 2021. The results also include results for trip spike blanks, field blanks, and a duplicate collected during the two sampling events. The results provided in this report were analyzed by Dr. James McCord and Dr. Mark Strynar at ORD's laboratory in Research Triangle Park, NC. Sample processing was initiated within 10 days of receiving each sample batch.

The current data report provides a simple representation and summary of the NTA results. Therefore, the description of methods and quality assurance are brief and high-level. As study partners/collaborators, we anticipate that NJ DEP and EPA Region 2 scientists will assist in these additional reports and publications.

**Methods in Brief.** Water samples were analyzed by ultra-performance liquid chromatography mass spectrometry (UPLC-MS) using methods described within our Laboratory Quality Assurance Project Plan<sup>1,2</sup> and McCord *et al.* 2019<sup>3</sup>.

In brief, water samples (500 mL) were filtered and then extracted using a WAX solid phase extraction cartridge. PFAS was removed from the cartridge in methanol and the volume reduced to 1 mL under a gentle stream of dry nitrogen. An aliquot of the 1 mL concentrated sample was injected into a Thermo Fisher Scientific<sup>TM</sup> Vanquish<sup>TM</sup> UPLC coupled to a Thermo Fisher Scientific<sup>TM</sup> Orbitrap Fusion<sup>TM</sup> MS. Samples were not diluted.

Samples were initially processed using targeted analysis methods with authentic standards to determine concentrations of a group of legacy PFAS compounds as reported in NJ DEP Report #10<sup>4</sup>. PFAS were then analyzed using NTA methods reported in this data report. NTA provides two important measurements. The first is a tentative identification of PFAS compounds detected in the sample based on a combination of mass spectral data along with patterns of fragmentation compared to on-line and in-house mass-spectral libraries. These compounds are considered to be likely PFAS (or breakdown products) based on diagnostic mass spectrometry information. In the absence of chemical standards, assignment of features is based on a preponderance of evidence. Analytes in each sample and process blank were identified to various levels of confidence depending on the combined evidence from manual examination of MS/MS fragmentation spectra and/or comparison with mass spectral libraries.

The second measurement is an indication of the relative abundance of the PFAS present in the sample. The MS detector provides integrated peak areas for the chromatogram of the compound mass (+/- 5 ppm) at the specified retention time. The peak area counts are proportional to the mass of PFAS in the sample. Since the sample and injection volume are held constant, the peak area counts are also proportional to concentration, although the relationship varies based on compound.

It is important to understand how NTA results differ from those produced during routine laboratory targeted analysis. Without a standard curve to calibrate the relationship between peak

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<sup>1</sup>National Exposure Research Laboratory, Quality Assurance Project Plan: Detection, Evaluation and Assignment of Multiple Poly and Per-fluoroalkyl Substances (PFAS) in environmental media from an industrialized area of New Jersey. Prepared for New Jersey Department of Environmental Protection (NJ DEP), D-EMMD-IEIB-010-QAPP-01, September 14, 2017.

<sup>2</sup>National Exposure Research Laboratory, Quality Assurance Project Plan: Detection, Evaluation and Assignment of Multiple Poly and Per-fluoroalkyl Substances (PFAS) in environmental media from an industrialized area of New Jersey. Prepared for New Jersey Department of Environmental Protection (NJ DEP) Amendment 2, D-EMMD-0031345-QO-1-2, September 3, 2019

<sup>3</sup>McCord, J., Strynar, M. Identifying Per- and Polyfluorinated Chemical Species with a Combined Targeted and Non-Targeted-Screening High-Resolution Mass Spectrometry Workflow. *J. Vis. Exp.* (146), e59142, doi:10.3791/59142 (2019).  
<https://www.jove.com/video/59142/identifying-per-polyfluorinated-chemical-species-with-combined>

<sup>4</sup> NJ DEP Report #10. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #10: Targeted Analysis of PFAS in Wastewater and Groundwater Samples Collected at the Solvay Specialty Polymers Plant in West Deptford, N.J. U.S.EPA/ORD, June 17, 2021.

area and a mass or concentration value, the peak area counts alone should be considered a semi-quantitative indicator of relative abundance. Analyte peak areas can be compared between samples in a sample set to obtain relative concentrations but cannot be directly compared between analytes because of fundamental differences in spectral characteristics between compounds. Our experience indicates that measured abundances for PFAS are four to six orders of magnitude higher than the ppt concentration (e.g.,  $1e7 \sim 100$  ppt), but even this relative difference can vary by several orders of magnitude between compounds. Peak area counts are expected to have much greater inherent sampling and analytical variability, which may become evident in reproducibility assessments. For example, it is possible for field duplicates to differ by two or three-fold or more, and laboratory replicates to have greater variability than typically observed in routine laboratory analysis. Any application of NTA results should consider this inherently greater uncertainty.

## Summary of Results

### Compound Identification

Across all the samples, we detected and tentatively identified 141 different PFAS listed in Table 2. Chemical information, such as the chemical formula, retention time (RT), and theoretical neutral monoisotopic mass of the most likely chemical identity are provided. The analyst grouped these compounds into 6 identified major classes with similar characteristics discussed in this report plus internal standards. Several additional “unknown” classes were identified at lower confidence and are not reported. The chemical classes are loosely defined by the major structural motifs of the chemicals identified. Some of the compound classes are familiar such as the legacy perfluorinated acid compounds (such as PFNA), the congener series named Chloro-Perfluoro-Polyether-Carboxylates (CIPFPECA) reported in previous data reports, and non-chlorinated fluoroether analogs to CIPFPECA.

Confidence applied by the analyst to each compound are also provided in Table 2. Analyst ratings are further defined in Appendix A. The analyst manually checked all compounds included in this data report. An additional 178 compounds were identified to formula or mass only. These compounds are not included in this report.

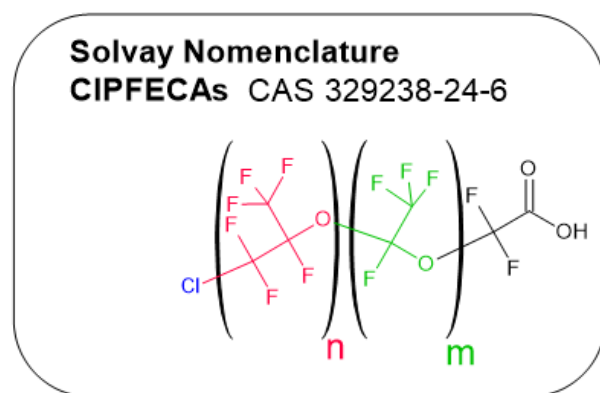
**Table 2. PFAS Tentatively Identified in Solvay-related Samples by UPCL-MS Non-targeted Analysis (continued next page).**

Chem. Ref. #	Report Class Name	Tentatively Identified Compound Name	Report Class	Formula	Monoisotopic Mass (g/mol)	RT	Analyst Confidence
1	Legacy Compounds	Perfluoropentanoic acid (PFPeA)	1a	HC5O2F9	263.9833	2.73	1
2	Legacy Compounds	Perfluorohexanoic acid (PFHxA)	1a	HC6O2F11	313.9801	4.09	1
3	Legacy Compounds	Perfluoroheptanoic acid (PFHpA)	1a	HC7O2F13	363.9768	5.15	1
4	Legacy Compounds	Perfluorooctanoic acid (PFOA)	1a	HC8O2F15	413.9738	6.03	1
5	Legacy Compounds	Perfluorononanoic acid (PFNA)	1a	HC9O2F17	463.9706	6.76	1
6	Legacy Compounds	Perfluorodecanoic acid (PFDA)	1a	HC10O2F19	513.9676	7.49	1
7	Legacy Compounds	Perfluoroundecanoic acid (PFUdA)	1a	HC11O2F21	563.9640	8.14	1
8	Legacy Compounds	Perfluoro-1-butanesulfonic acid (PFBS)	1b	HC4O3F9S	299.9505	3.79	1
9	Legacy Compounds	Perfluoro-1-pentanesulfonate (PFPeS)	1b	HC5O3F11S	349.9468	5.02	1
10	Legacy Compounds	Perfluoro-1-hexanesulfonic acid (PFHxS)	1b	HC6O3F13S	399.9444	5.80	1
11	Legacy Compounds	Perfluoro-1-heptanesulfonate (PFHpS)	1b	HC7O3F15S	449.9407	6.83	1
12	Legacy Compounds	Perfluoro-1-octanesulfonic acid (PFOS)	1b	HC8O3F17S	499.9380	7.57	1
13	Legacy Compounds	Perfluoro-1-nonanesulfonate (PFNS)	1b	HC9O3F19S	549.9346	8.24	1
14	Legacy Compounds	Perfluoro-1-decanesulfonic acid (PFDS)	1b	HC10O3F21S	599.9308	8.88	1
15	Legacy Compounds	6:2 Fluorinated telomer sulfonate	1c	H5C8O3F13S	427.9742	5.76	1
16	Legacy Compounds	4:2 Fluorinated telomer sulfonate	1c	H5C6O3F9S	327.9815	3.79	1
17	Chlorinated Fluoroethers	CIPFPECA(0,1)	2a	HC8O4F14Cl	461.9342	6.60	1
18	Chlorinated Fluoroethers	CIPFPECA(0,2)	2a	HC11O5F20Cl	627.9201	8.53	1
19	Chlorinated Fluoroethers	CIPFPECA(1,1)	2a	HC10O5F18Cl	577.9234	8.02	1
20	Chlorinated Fluoroethers	CIPFPECA(2,0)	2a	HC9O5F16Cl	527.9263	7.46	1
21	Chlorinated Fluoroethers	CIPFPECA(1,0)	2a	HC7O4F12Cl	411.9374	5.98	1
22	Chlorinated Fluoroethers	CIPFPECA(0,0)	2a	HC5O3F8Cl	295.9488	3.57	2b
23	Chlorinated Fluoroethers	CIPFPECA(2,0), with ClCF2CF2O tail	2b	HC8O5F14Cl	477.9289	6.86	2b
24	Chlorinated Fluoroethers	CIPFPECA(0,1)+C2F4	2b	HC10O4F18Cl	561.9277	7.71	2b
25	Chlorinated Fluoroethers	CIPFPECA(0,1), without ether linkage	2b	HC8O3F14Cl	445.9391	6.21	3
26	Chlorinated Fluoroethers	Cl-C3F6O-CF2O-CF2-COOH	2b	HC6O4F10Cl	361.9404	5.13	2b
27	Chlorinated Fluoroethers	CIPFPECA(0,2), without one ether	2b	HC11O4F20Cl	611.9247	8.13	3
28	Chlorinated Fluoroethers	CIPFPECA with C3H6 moiety	2c	H7C14O6F22Cl	723.9584	5.99	3
29	Chlorinated Fluoroethers	Cl(C2F4O)6 + C6H12O	2c	H13C18O7F24Cl	831.9965	6.86	3
30	Chlorinated Fluoroethers	CIPFPECA(1,1) with Cl <> F replacement	2c	HC10O5F17Cl2	593.8935	8.18	3
31	Chlorinated Fluoroethers	CIPFPECA(2,0), with H <> F exchange	2c	H2C9O5F15Cl	509.9356	6.86	2b
32	Chlorinated Fluoroethers	unknown	2c	H13C11O2F10Cl	402.0445	9.20	4
33	Chlorinated Fluoroethers	unknown	2c	H4C7O2FCl	173.9884	1.79	4
34	NonChlorinated Fluoroethers	HPFPECA(1,1)	3a	H2C10O5F18	543.9622	7.19	1
35	NonChlorinated Fluoroethers	HPFPECA(0,1)	3a	H2C8O4F14	427.9730	5.88	1
36	NonChlorinated Fluoroethers	HPFPECA(1,0)	3a	H2C7O4F12	377.9760	5.07	1
37	NonChlorinated Fluoroethers	HPFPECA(2,0)	3a	H2C9O5F16	493.9649	7.00	1
38	NonChlorinated Fluoroethers	HPFPECA(0,2)	3a	H2C11O5F20	593.9585	7.84	1
39	NonChlorinated Fluoroethers	H-(CF2CF2O)3-(CF2O)-CF2-COOH	3b	H2C9O6F16	509.9598	7.22	1b
40	NonChlorinated Fluoroethers	H-(CF2CF2O)2-CF2-COOH	3b	H2C6O4F10	327.9793	3.90	2b
41	NonChlorinated Fluoroethers	HPFPECA(2,0), with HCF2CF2O tail	3b	H2C8O5F14	443.9678	6.20	2b
42	NonChlorinated Fluoroethers	H-(CF2CF2O)-(CF2O)4-CF2-COOH	3b	H2C8O7F14	475.9579	6.81	2b
43	NonChlorinated Fluoroethers	H-(CF2CF2O)-(CF2O)2-CF2-COOH	3b	H2C6O5F10	343.9741	4.68	2b
44	NonChlorinated Fluoroethers	FPFPECA(2,0)	3b	HC9O5F17	511.9554	7.27	1
45	NonChlorinated Fluoroethers	H-(CF2CF2O)2-(CF2O)-CF2-COOH	3b	H2C7O5F12	393.9709	5.52	2b
46	NonChlorinated Fluoroethers	Polyfluoroether alcohol	3c	H14C11O4F10	400.0730	7.10	3

Chem. Ref. #	Report Class Name	Tentatively Identified Compound Name	Report Class	Formula	Monoisotopic Mass (g/mol)	RT	Analyst Confidence
47	NonChlorinated Fluoroethers	OH-C2F3H-(C2F4O)3-CF2COOH	3c	H3C1007F17	557.9595	6.23	2b
48	NonChlorinated Fluoroethers	Polyfluoroether alcohol	3c	H3C8O6F13	441.9720	4.80	3
49	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=5)	4a	H14C12O3F10S	428.0504	4.78	3
50	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=6)	4a	H16C14O3F12S	492.0633	5.64	3
51	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=4)	4a	H12C10O3F8S	364.0381	4.04	3
52	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=7)	4a	H18C16O3F14S	556.0748	6.25	3
53	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=3)	4a	H10C8O3F6S	300.0255	2.24	3
54	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=2)	4a	H8C6O3F4S	236.0131	0.95	3
55	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=8)	4a	H20C18O3F16S	620.0873	6.88	3
56	PVDF Sulfonates	H-(C2F2H2)n-C2H2-SO3H (n=9)	4a	H22C20O3F18S	684.1003	7.24	3
57	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=5)	4b	H12C10O3F10S	402.0346	3.79	2b
58	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=4)	4b	H10C8O3F8S	338.0224	2.36	2b
59	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=6)	4b	H14C12O3F12S	466.0473	4.84	2b
60	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=3)	4b	H8C6O3F6S	274.0099	1.52	2b
61	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=7)	4b	H16C14O3F14S	530.0600	5.68	2b
62	PVDF Sulfonates	H-(C2F2H2)n-SO3H (n=8)	4b	H18C16O3F16S	594.0717	6.25	2b
63	PVDF Sulfonates	H-(C2F2H2)n-C3F6-SO3H (n=3)	4c	H8C9O3F12S	424.0003	5.38	3
64	PVDF Sulfonates	H-(C2F2H2)n-C3F6-SO3H (n=2)	4c	H6C7O3F10S	359.9878	4.38	3
65	PVDF Sulfonates	H-(C2F2H2)n-C3F6-O3SH (n=4)	4c	H10C11O3F14S	488.0132	6.15	3
66	PVDF Sulfonates	H-(C2F2H2)n-C3F6-SO3H (n=1)	4c	H4C5O3F8S	295.9753	3.04	3
67	PVDF Sulfonates	H-(C2F2H2)n-C3F6-SO3H (n=5)	4c	H12C13O3F16S	552.0261	6.80	3
68	PVDF Sulfonates	H-(C2F2H2)n-C3F6-SO3H (n=6)	4c	H14C15O3F18S	616.0383	6.84	3
69	PVDF Sulfonates	(C2F2H2)n-SO3 (n=5)	4d	H10C10O3F10S	400.0190	4.42	2b
70	PVDF Sulfonates	(C2F2H2)n-SO3 (n=6)	4d	H12C12O3F12S	464.0319	5.58	2b
71	PVDF Sulfonates	(C2F2H2)n-SO3 (n=7)	4d	H14C14O3F14S	528.0449	5.60	2b
72	PVDF Sulfonates	(C2F2H2)n-SO3 (n=4)	4d	H8C8O3F8S	336.0065	2.82	2b
73	PVDF Sulfonates	(C2F2H2)n-SO3 (n=8)	4d	H16C16O3F16S	592.0568	6.36	2b
74	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=3)	4e	H16C11O3F6S	342.0721	4.03	3
75	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=2)	4e	H14C9O3F4S	278.0602	2.95	3
76	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=4)	4e	H18C13O3F8S	406.0847	4.92	3
77	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=1)	4e	H12C7O3F2S	214.0475	1.77	3
78	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=5)	4e	H20C15O3F10S	470.0976	5.83	3
79	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=6)	4e	H22C17O3F12S	534.1102	6.32	3
80	PVDF Sulfonates	(C2H2F2)n-C5H10-SO3 (n=7)	4e	H24C19O3F14S	598.1220	6.87	3
81	PVDF Sulfonates	(C2H2F2)n-C3H6-SO3 (n=3)	4f	H12C9O3F6S	314.0413	3.53	3
82	PVDF Sulfonates	(C2H2F2)n-C3H6-SO3 (n=4)	4f	H14C11O3F8S	378.0534	4.07	3
83	PVDF Sulfonates	(C2H2F2)n-C3H6-SO3 (n=6)	4f	H18C15O3F12S	506.0789	6.24	3
84	PVDF Sulfonates	(C2H2F2)n-C3H6-SO3 (n=5)	4f	H16C13O3F10S	442.0658	5.56	3
85	PVDF Sulfonates	(C2H2F2)n-C3H6-SO3 (n=7)	4f	H20C17O3F14S	570.0907	6.92	3
86	PVDF Sulfonates	H(C2H2F2)n-C3H6-SO3H (n=3)	4g	H14C9O3F6S	316.0562	3.54	3
87	PVDF Sulfonates	H(C2H2F2)n-C3H6-SO3H (n=2)	4g	H12C7O3F4S	252.0438	1.65	3
88	PVDF Sulfonates	H(C2H2F2)n-C3H6-SO3H (n=6)	4g	H20C15O3F12S	508.0943	6.22	3
89	PVDF Sulfonates	H(C2H2F2)n-C3H6-SO3H (n=7)	4g	H22C17O3F14S	572.1057	6.77	3
90	PVDF Sulfates	(C2F2H2)n-SO4 (n=4)	5a	H8C8O4F8S	352.0018	4.00	2b
91	PVDF Sulfates	(C2F2H2)n-SO4 (n=6)	5a	H12C12O4F12S	480.0268	5.70	2b
92	PVDF Sulfates	(C2F2H2)n-SO4 (n=5)	5a	H10C10O4F10S	416.0141	5.54	2b
93	PVDF Sulfates	(C2F2H2)n-SO4 (n=3)	5a	H6C6O4F6S	287.9893	2.33	3
94	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=4)	5b	H10C8O4F8S	354.0168	3.22	2b
95	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=5)	5b	H12C10O4F10S	418.0298	4.46	2b



Chem. Ref. #	Report Class Name	Tentatively Identified Compound Name	Report Class	Formula	Monoisotopic Mass (g/mol)	RT	Analyst Confidence
96	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=6)	5b	H14C12O4F12S	482.0425	5.42	2b
97	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=3)	5b	H8C6O4F6S	290.0049	1.88	2b
98	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=2)	5b	H6C4O4F4S	225.9921	0.96	2b
99	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=7)	5b	H16C14O4F14S	546.0550	6.14	2b
100	PVDF Sulfates	H-(C2F2H2)n-SO4H (n=8)	5b	H18C16O4F16S	610.0663	6.75	2b
101	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=2)	5c	H6C7O4F10S	375.9824	4.44	3
102	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=3)	5c	H8C9O4F12S	439.9954	5.32	3
103	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=1)	5c	H4C5O4F8S	311.9703	3.14	3
104	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=4)	5c	H10C11O4F14S	504.0080	6.07	2b
105	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=5)	5c	H12C13O4F16S	568.0197	6.72	3
106	PVDF Sulfates	H-(C2F2H2)n-C3F6-SO4H (n=6)	5c	H14C15O4F18S	632.0329	7.26	3
107	PVDF Sulfates	(C2H2F2)n-C5H10-SO4 (n=3)	5d	H16C11O4F6S	358.0673	2.63	3
108	PVDF Sulfates	(C2H2F2)n-C5H10-SO4 (n=5)	5d	H20C15O4F10S	486.0922	5.20	3
109	PVDF Sulfates	(C2H2F2)n-C5H10-SO4 (n=4)	5d	H18C13O4F8S	422.0797	3.70	3
110	PVDF Sulfates	(C2H2F2)n-C5H10-SO4 (n=2)	5d	H14C9O4F4S	294.0548	1.54	3
111	PVDF Sulfates	(C2H2F2)n-C7H12-SO4 (n=3)	5e	H18C13O4F6S	384.0829	3.85	3
112	PVDF Sulfates	(C2H2F2)n-C7H12-SO4 (n=4)	5e	H20C15O4F8S	448.0954	4.55	3
113	PVDF Sulfates	(C2H2F2)n-C7H12-SO4 (n=5)	5e	H22C17O4F10S	512.1082	5.58	3
114	PVDF Sulfates	(C2H2F2)n-C7H12-SO4 (n=6)	5e	H24C19O4F12S	576.1201	6.19	3
115	PVDF Sulfates	H(C2H2F2)n-SO5H (n=4, monoether)	5f	H10C8O5F8S	370.0118	2.84	3
116	PVDF Sulfates	H(C2H2F2)n-SO5H (n=5, monoether)	5f	H12C10O5F10S	434.0246	3.54	3
117	PVDF Sulfates	H(C2H2F2)n-SO5H (n=6, monoether)	5f	H14C12O5F12S	498.0373	5.27	3
118	PVDF Sulfates	H(C2H2F2)n-SO5H (n=8, monoether)	5f	H18C16O5F16S	626.0618	5.95	3
119	PVDF Sulfates	H(C2H2F2)n-SO5H (n=7, monoether)	5f	H16C14O5F14S	562.0492	5.62	3
120	PVDF Sulfates	H(C2H2F2)n-C2H2O-SO4H (n=5)	5g	H14C12O5F10S	460.0402	2.32	3
121	PVDF Sulfates	H(C2H2F2)n-C2H2O-SO4H (n=6)	5g	H16C14O5F12S	524.0529	1.60	3
122	PVDF Sulfates	H(C2H2F2)n-C2H2O-SO4H (n=7)	5g	H18C16O5F14S	588.0650	3.80	3
123	PVDF Sulfates	H(C2H2F2)n-C2H2O-SO4H (n=4)	5g	H12C10O5F8S	396.0280	1.56	3
124	PVDF Sulfates	H(C2H2F2)n-C2H2O-SO4H (n=8)	5g	H20C18O5F16S	652.0778	3.42	3
125	PVDF Sulfates	H(C2H2F2)n-C2H4O-SO4H (n=7)	5h	H18C14O5F10S	488.0716	5.41	3
126	PVDF Sulfates	H(C2H2F2)n-C2H4O-SO4H (n=5)	5h	H14C10O5F8S	398.0433	2.91	3
127	PVDF Sulfates	H(C2H2F2)n-C2H4O-SO4H (n=6)	5h	H16C12O5F10S	462.0560	4.06	3
128	PVDF Sulfates	H(C2H2F2)n-C2H4O-SO4H (n=4)	5h	H12C8O5F6S	334.0308	1.73	3
129	PVDF Sulfates	H(C2H2F2)n-C2H4O-SO4H (n=8)	5h	H20C18O5F18S	690.0744	6.53	3
130	PVDF Carboxylates	H-(C2F2H2)n-C3F6-COOH (n=1, oxidized HFPO+PVDF)	6a	H4C6O2F8	260.0085	1.98	3
131	PVDF Carboxylates	H-(C2F2H2)n-C3F6-COOH (n=3)	6a	H8C10O2F12	388.0330	4.42	3
132	PVDF Carboxylates	H-(C2F2H2)n-C3F6-COOH (n=2)	6a	H6C8O2F10	324.0206	3.18	3
133	PVDF Carboxylates	H-(C2F2H2)n-C3F6-COOH (n=4)	6a	H10C12O2F14	452.0459	5.36	3
134	PVDF Carboxylates	H-(C2F2H2)n-CF2-COOH (n=4)	6b	H10C10O2F10	352.0516	3.86	3
135	PVDF Carboxylates	H-(C2F2H2)n-CF2-COOH (n=2)	6b	H6C6O2F6	224.0273	1.54	3
136	PVDF Carboxylates	H-(C2F2H2)n-CF2-COOH (n=6)	6b	H14C14O2F14	480.0772	5.81	3
137	PVDF Carboxylates	H-(C2F2H2)n-CF2-COOH (n=5)	6b	H12C12O2F12	416.0645	4.48	3
138	PVDF Carboxylates	H-(C2F2H2)n-CF2-COOH (n=3)	6b	H8C8O2F8	288.0397	1.92	3
139	PVDF Carboxylates	H-(C2F2H2)n-COOH (n=4)	6c	H10C9O2F10	340.0507	4.78	2b
140	PVDF Carboxylates	H-(C2F2H2)n-COOH (n=5)	6c	H12C11O2F10	366.0675	8.91	2b
141	PVDF Carboxylates	H-(C2F2H2)n-COOH (n=6)	6c	H14C13O2F12	430.0801	8.59	2b

**Figure 2. Generic Structure of Chloro-Perfluoro-Polyether-Carboxylate (CIPFPECA).**

Solvay refers to the CIPFPECA compounds as monofunctional surfactants (MFS) with the generic structure shown in Figure 2. The terminal Cl-C<sub>2</sub>F<sub>6</sub>O is treated as an additional “n” group with a Cl at the end. According to Solvay nomenclature the (n) is the propyl group and the (m) the ethyl group. Analysis of soils in Report #2<sup>5</sup> identified nine congeners with m and n varying from 0 to 3. The analysis of well samples in Report #7<sup>6</sup> identified 6 congeners with m and

n varying from 0 to 2. Note that the “m” and “n” in this report are positionally switched from compound representations shown in previous reports<sup>5,6</sup> to be consistent with Solvay nomenclature. To assist with comparison to earlier reports, the naming conventions used by Solvay and EPA for these chemicals are provided in Table 3 with additional formula information about these chemicals available in Appendix B.

**Table 3. Molecular Formula, Naming Conventions, and Monoisotopic Mass of Chloro-Perfluoro-Polyether-Carboxylate (CIPFPECA) Compounds.**

Formula	Solvay Name	EPA Name	M-H Monoisotopic Mass (g/mol)
C <sub>8</sub> H Cl F <sub>14</sub> O <sub>4</sub>	MFS-N2	Cl-PFECA 0,1	460.9267
C <sub>11</sub> H Cl F <sub>20</sub> O <sub>5</sub>	MFS-N3	Cl-PFECA 0,2	626.912
C <sub>14</sub> H Cl F <sub>26</sub> O <sub>6</sub>	MFS-M4	Cl-PFECA 0,3	792.8974
C <sub>17</sub> H Cl F <sub>32</sub> O <sub>7</sub>	MFS-N5	Cl-PFECA 0,4	958.8827
C <sub>8</sub> H Cl F <sub>16</sub> O <sub>3</sub>	MFS-M3	Cl-PFECA 1,1	576.9152
C <sub>13</sub> H Cl F <sub>24</sub> O <sub>6</sub>	MFS-M4	Cl-PFECA 1,2	742.9006

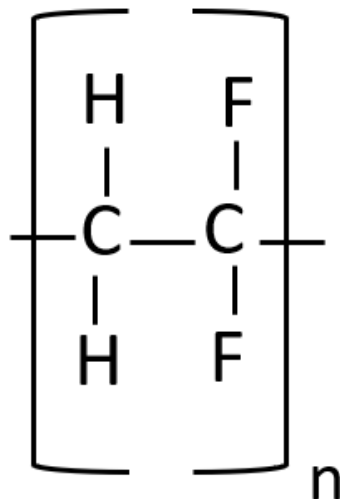
The primary polymer product made at the Solvay facility is polyvinylidene fluoride, also known as polyvinylidene disulfide, and is generally referred to by the four-letter acronym PVDF. PVDF is a polymer that belongs to the thermoplastic category of plastics that is composed of long chains of repeating molecule carbon/fluorine units that are linked together through a synthesis reaction at high temperature. PVDF can be made into a variety of products including sheets, films, pipes, containers, specialized equipment and individual items, and can be used as a solid or liquid coating.

<sup>5</sup> NJ DEP Report #2. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #2: Non-targeted Analysis of PFAS in Soil and Vegetation. U.S.EPA/ORD, March 8, 2019.

<sup>6</sup> NJ DEP Report #7. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #7: Non-targeted Analysis of PFAS in Water Samples Collected from Wells with Point of Entry Treatment. U.S.EPA/ORD, April 24, 2020

The general structure of PVDF compounds is shown in Figure 3. The carbon chain alternates between fluorines and hydrogens in these compounds as opposed to fully fluorinated.

**Figure 3. Generic Structure of Polyvinylidene compounds (PVDF).**



Several classes of PVDF byproduct compounds with different end groups that appear to result from the chemical processing were identified in the water samples. Table 2 lists PVDF compounds identified in classes that were developed by the analyst for this report. The PVDF classes are distinguished by type of acidic head group, including carboxylates, sulfonates, or sulfates. These various compounds classes are not widely reported, although they have been observed in some samples at this location as well as in surface water samples collected elsewhere that have been impacted by PVDF polymer production<sup>7</sup>. These compounds are hypothesized to originate from early termination of PVDF polymerization to yield soluble byproducts and can be identified in both alkyl and alkene forms. The primary compounds have one or more isomers from repeating unit orientation and are distinguished by retention time but are expected to have similar intrinsic properties.

In addition to their assigned major class (1-6) compounds within classes may also be assigned a letter (a-g) reflecting their association within a homologous series within that class. For example, within major class 4, a polymeric series was detected with formula  $\text{H}-(\text{C}_2\text{F}_2\text{H}_2)_n-\text{C}_2\text{H}_2-\text{SO}_3\text{H}$  with  $n$  ranging from 2 to 9, all of which were assigned to class 4a. Subclass letters within a major class are only relevant to that class. There is no association of lettered subclasses between major classes.

## Abundance of Compounds

### Reporting Limits

The NTA data generated by UPLC/MS were considered as a “detect” when acceptable chromatographic peaks and spectra were evident. Note that in previous data reports, samples without a detectable peak were reported as “ND” or not detected. Updates to the LCMS processing software now report the background ND threshold when no peak is detected instead of an ND value. As a result, all of the samples, as well as laboratory and field blanks had some level of peak area detected as analytical “noise” and there is no category of “ND”. A post-processing screening technique was applied that removes low level noise to determine the peak area reporting limit (RL). A lower reporting limit that accounts for this background noise by statistical analysis of the peak areas in the laboratory blanks according to Equation 1.

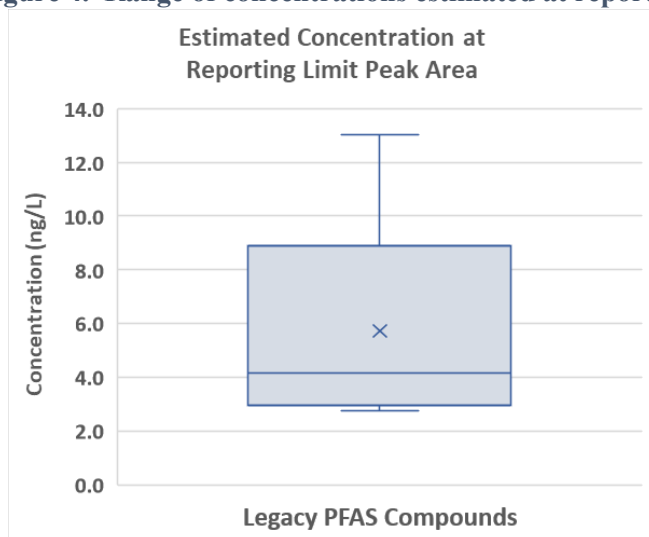
<sup>7</sup> Newton, S., R. McMahan, J.A. Stoeckel, M. Chislock, A. Lindstrom, M. Strynar. Novel polyfluorinated compounds identified using high resolution mass spectrometry downstream of manufacturing facilities near Decatur, Alabama. Env. Sci. Tech. 2017. <https://pubs.acs.org/doi/abs/10.1021/acs.est.6b05330>.

***Eq 1. Reporting Limit (RL) = Average [Laboratory blanks] + 5 x STD [blanks]***

The equation produces a lower threshold above which there is a high probability of positive presence of an analyte within the sample given the standard deviation multiplier. Samples with peak areas less than this threshold are reported as “<RL”. In this case, peak areas were detected but are probably not present in measurable amounts if they could be quantitated with known standards. This technique has been previously applied in NTA data reports to NJDEP. The technique may screen out some contamination that may have occurred during sampling or laboratory analysis.

NTA analysis was also performed on the calibration standards for 9 legacy analytes (PFPeA, PFHxA, PFHpA, PFOA, PFNA, PFDA, PFBS, PFHxS, and PFOS) used in targeted analysis allowing a check on our method for establishing lower reporting limits. Similar to targeted analysis, the NTA peak areas of the calibration standards were regressed with their known concentrations allowing computation of either concentrations from peak area or peak area from concentration. The regressions for the nine analytes had  $R^2 > 0.99$  except for PFHxS that was not well correlated with  $R^2 = 0.78$ .

**Figure 4. Range of concentrations estimated at reporting level peak area for nine legacy compounds.**



Inputting the reporting limit peak areas computed with equation 1 into these regressions produced a range of reporting limit concentrations from 3 to 13 ng/L with mean of 4 and median of 6 ng/L (Figure 4). The established limit of quantitation for these same compounds in targeted analysis was 5 ng/L based on calibration curves as reported in NJDEP Report #10<sup>4</sup>.

The reporting limit computation produced reasonably similar results for previously quantitated legacy analytes, albeit with the expected variability among analytes inherent in NTA. The thresholds for

reporting are, therefore, consistent with thresholds from established quantitation techniques. This computation was applied to establish reporting limits for all of the compounds, although it is not known if the other compounds relate to minimum quantitation levels as well as the legacy compounds did, or at what concentrations they may represent for those compounds. Note that peak area reporting limit thresholds vary widely among analytes, even within the same compound class, ranging from 5,500 to 6,000,000.

### ***PFAS in Samples***

To assist interpretation of relative abundance of PFAS compounds within the wide variation in peak areas associated with individual analytes, the peak areas were scaled relative to their reporting limit using the following ratio (equation 2).

$$\text{Eq 2. Scaled Peak Area} = \frac{\text{Peak Area of Sample}}{\text{Peak Area Reporting Limit}}$$

The reported values are a relative abundance ratio comparison with the assumed minimum signal threshold for the given compound. These values are indicators of the relative intensity of the signal but should not be taken to represent a concentration as they are not produced based on known calibration standards. NTA results expressed as the Scaled Peak Area are presented grouped by compound class in Tables 4-9. The peak areas at the reporting limit for each compound are provided in the tables allowing computation of sample/analyte peak area as reported in earlier data reports. The Scaled Peak Area has been rounded and is reported to the nearest whole integer. Raw peak area may be obtained following Eq 2 for comparison with previous NTA reports.

The general abundance of legacy PFAS as indicated by the Scaled Peak Areas in Table 4 are of the same order of magnitude as legacy concentrations determined with targeted analysis. PFOA and PFNA were found in relatively high abundance in multiple samples in NTA consistent with concentration results reported for targeted analysis in NJDEP Report #10<sup>4</sup>. NTA found two additional legacy PFAS compounds in relatively higher abundance at various waste discharge locations within the plant including Perfluoroundecanoic acid (PFUdA) and 6:2 fluorinated telomer sulfonate. The relative abundance of PFUdA in Table 4 is particularly high and may be one compound where the Scaled Peak Area exaggerates the abundance due to the unusually low reporting limit for this compound, and low sensitivity for the response. Scaled peak areas are similar to PFHpA which was quantitated at 26-88 ng/L in targeted analysis at the same locations. Targeted analysis concentrations should always be used when available.

Previous data reports for NTA analysis of soil<sup>5</sup>, sediment<sup>8</sup>, and wells<sup>7</sup> in the vicinity of the Solvay plant provided peak areas for the congener series named Chloro-Perfluoro-Polyether-Carboxylates (CIPFPECA). Table 5 provides NTA results expressed as the Scaled Peak Area for these compounds in the samples collected from the waste discharge stream from the Solvay facility. Three congeners including (0,1), (1,1) and (0,2) made up the bulk of peak area in soils, vegetation, sediments, and wells. These same congeners also made up the bulk of the peak area in samples collected from the waste stream of the Solvay plant. There was no abundance of CIPFPECA's greater than the reporting limit at the V770 post process treatment location within the Solvay plant before discharge to GCUA, although some was present in the combined sewer discharge from the plant (GCUA-PS).

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<sup>8</sup> NJ DEP Report #5. Detection, Evaluation, and Assignment of PFAS in Environmental Media from an Industrialized Area of New Jersey. Laboratory Data Report #2: Non-targeted Analysis of PFAS in Sediment. U.S.EPA/ORD, April 23, 2020

**Table 4. Scaled Peak Area of Samples Calculated as the Ratio of the Sample Peak Area to the Analyte Reporting Limit Peak Area for Legacy PFAS Compounds (Report Class 1) Determined with Non-targeted Analysis.**

Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area Legacy PFAS Compounds														
				INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
1	Perfluoropentanoic acid (PFPeA)	1a	239,924	10	11	<RL	5	3	2	1	<RL	1	<RL	4	1	<RL	<RL	<RL
2	Perfluorohexanoic acid (PFHxA)	1a	266,425	37	42	1	20	10	4	2	<RL	12	<RL	20	8	<RL	<RL	<RL
3	Perfluoroheptanoic acid (PFHpA)	1a	2,433,021	11	12	<RL	6	3.1	1	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
4	Perfluorooctanoic acid (PFOA)	1a	674,112	383	384	<RL	193	187	164	103	<RL	26	1	7	3	<RL	<RL	<RL
5	Perfluorononanoic acid (PFNA)	1a	2,614,514	606	607	<RL	276	267	170	88	<RL	44	4	2	1	<RL	<RL	<RL
6	Perfluorodecanoic acid (PFDA)	1a	188,070	83	91	15	43	29	15	7.2	<RL	4	<RL	1	<RL	<RL	<RL	<RL
7	Perfluoroundecanoic acid (PFUdA)	1a	5,468	5,420	5,610	2	3,050	1,680	1,670	66	2	597	180	4	1	<RL	<RL	1
8	Perfluoro-1-butanefulfonic acid (PFBS)	1b	498,634	1	1	<RL	<RL	<RL	3	3	<RL	<RL	<RL	22	2	<RL	<RL	<RL
9	Perfluoro-1-pentanesulfonate (PFPeS)	1b	15,495	13	12	<RL	13	5	48	7	<RL	1	<RL	18	<RL	<RL	<RL	<RL
10	Perfluoro-1-hexanesulfonic acid (PFHxS)	1b	5,797,158	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
11	Perfluoro-1-heptanesulfonate (PFHpS)	1b	17,121	<RL	<RL	<RL	1.7	4	6	6	<RL	<RL	<RL	5	<RL	2	<RL	<RL
12	Perfluoro-1-octanesulfonic acid (PFOS)	1b	178,311	19	23	<RL	17	10	6	3	2	1	1	14	8	<RL	<RL	<RL
13	Perfluoro-1-nonanesulfonate (PFNS)	1b	32,017	<RL	<RL	<RL	<RL	2	2	3	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
14	Perfluoro-1-decanesulfonic acid (PFDS)	1b	26,634	<RL	<RL	<RL	<RL	2	2	4	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
15	6:2 Fluorinated telomer sulfonate	1c	207,865	130	133	<RL	52	27	149	104	<RL	243	12	5	<RL	<RL	<RL	<RL
16	4:2 Fluorinated telomer sulfonate	1c	14,373	9	9	<RL	3.8	4.9	42	16	<RL	2	<RL	<RL	<RL	<RL	<RL	<RL
<b>Reporting Class Sum</b>				6,721	6,935	18	3,680	2,234	2,284	412	3	931	199	101	26	2	0	1

**Table 5, Scaled Peak Area of Samples Calculated as the Ratio of Sample Peak Area to the Reporting Limit Peak Area for Chloro-Perfluoro-Polyether-Carboxylate (CIPFPECA) Compounds (Report Class 2) Determined with Non-targeted Analysis.**

Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area Chlorinated Fluoroethers														
				INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
17	CIPFPECA(0,1)	2a	3,264,476	867	867	21	378	492	7,200	28,000	<RL	604	132	6	<RL	<RL	<RL	<RL
18	CIPFPECA(0,2)	2a	170,238	98	93	6	112	183	19,900	11,600	<RL	103	239	1	<RL	<RL	<RL	<RL
19	CIPFPECA(1,1)	2a	750,979	15	15	1	14	36	1,770	2,550	<RL	9	12	<RL	<RL	<RL	<RL	<RL
20	CIPFPECA(2,0)	2a	178,154	38	41	4	31	105	3,230	8,760	<RL	24	26	<RL	<RL	<RL	<RL	<RL
21	CIPFPECA(1,0)	2a	80,029	98	89	1	45	59	971	2,140	<RL	154	13	1.9	<RL	<RL	<RL	<RL
22	CIPFPECA(0,0)	2a	104,968	119	130	<RL	61	5	115	287	<RL	492	1.4	3.0	<RL	<RL	<RL	<RL
23	CIPFPECA(2,0), with ClCF2CF2O tail	2b	58,603	107	105	6	54	117	3,560	8,520	<RL	98	39	<RL	<RL	<RL	<RL	<RL
24	CIPFPECA(0,1)+C2F4	2b	48,614	24	26	2	21	58	2,720	7,100	<RL	14	12	<RL	<RL	<RL	<RL	<RL
25	CIPFPECA(0,1), without ether linkage	2b	53,860	114	101	1	46	64	1,780	2,910	<RL	173	16	<RL	<RL	<RL	<RL	<RL
26	Cl-C3F6O-CF2O-CF2-COOH	2b	28,625	99	103	1	49	51	1,920	2,920	<RL	312	13	2	<RL	<RL	<RL	<RL
27	CIPFPECA(0,2), without one ether	2b	55,246	1.5	1.5	<RL	2.0	6	760	928	<RL	3.1	4.3	<RL	<RL	<RL	<RL	<RL
28	CIPFPECA with C3H6 moiety	2c	26,839	1.1	<RL	<RL	24	4	24,600	108	<RL	54	<RL	<RL	<RL	<RL	<RL	<RL
29	Cl(C2F4O)6 + C6H12O	2c	24,661	<RL	<RL	<RL	11	4	20,500	652	<RL	4	<RL	<RL	<RL	<RL	<RL	<RL
30	CIPFPECA(1,1) with Cl <> F replacement	2c	40,005	37	38	3	53	115	8,040	11,200	<RL	38	54	<RL	<RL	<RL	<RL	<RL
31	CIPFPECA(2,0), with H <> F exchange	2c	47,775	15	14	<RL	7	14	641	1,950	<RL	9	6	<RL	<RL	<RL	<RL	<RL
32	unknown	2c	49,255	14	17	<RL	1,210	4	62	6	<RL	1	<RL	4	<RL	1	<RL	<RL
<b>Reporting Class Sum</b>				1,660	1,655	47	2,521	1,319	97,817	89,636	0	2,093	568	18	0	1	0	0

**Table 6. Scaled Peak Area of Samples Calculated as the Ratio of Sample Peak Area to the Reporting Limit Peak Area for Non-chlorinated Fluoroether Compounds (Report Class 3) Determined with Non-targeted Analysis.**

Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area Non-chlorinated Fluoroethers														
				INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
34	HPFPECA(1,1)	3a	110,213	95	99	13	61	220	6,530	20,700	<RL	176	84	<RL	2	<RL	<RL	<RL
35	HPFPECA(0,1)	3a	83,290	2,210	1,310	2	1,050	1,100	11,800	6,210	<RL	1,290	237	56	7	<RL	<RL	<RL
36	HPFPECA(1,0)	3a	54,405	516	546	6	270	164	10,900	8,870	2	3,410	77	44	2	<RL	<RL	<RL
37	HPFPECA(2,0)	3a	108,773	56	56	1	26	31	1,090	2,520	<RL	53	15	<RL	<RL	<RL	<RL	<RL
38	HPFPECA(0,2)	3a	78,746	35	41	<RL	30	18	2,170	1,350	<RL	209	91	<RL	<RL	<RL	<RL	<RL
39	H-(CF <sub>2</sub> CF <sub>2</sub> O) <sub>3</sub> -(CF <sub>2</sub> O)-CF <sub>2</sub> -COOH	3b	58,660	163	175	<RL	118	39	51,400	3,140	<RL	217	51	1	<RL	<RL	<RL	<RL
40	H-(CF <sub>2</sub> CF <sub>2</sub> O) <sub>2</sub> -CF <sub>2</sub> -COOH	3b	72,580	282	286	2	152	158	4,440	8,340	1	1,270	68	15	3	<RL	<RL	<RL
41	HPFPECA(2,0), with HCF <sub>2</sub> CF <sub>2</sub> O tail	3b	81,250	178	159	2	77	58	3,440	2,860	<RL	264	22	1	<RL	<RL	<RL	<RL
42	H-(CF <sub>2</sub> CF <sub>2</sub> O)-(CF <sub>2</sub> O) <sub>4</sub> -CF <sub>2</sub> -COOH	3b	23,511	60	44	<RL	32	22	1,380	981	<RL	81	18	<RL	<RL	<RL	<RL	<RL
43	H-(CF <sub>2</sub> CF <sub>2</sub> O)-(CF <sub>2</sub> O) <sub>2</sub> -CF <sub>2</sub> -COOH	3b	50,144	75	80	<RL	34	11	277	75	<RL	619	<RL	3	<RL	<RL	<RL	<RL
44	FPFPECA(2,0)	3b	200,261	<RL	<RL	<RL	<RL	<RL	90	153	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL
45	H-(CF <sub>2</sub> CF <sub>2</sub> O) <sub>2</sub> -(CF <sub>2</sub> O)-CF <sub>2</sub> -COOH	3b	27,508	296	275	<RL	135	52	1,080	256	<RL	688	5	5	<RL	<RL	<RL	<RL
46	Polyfluoroether alcohol	3c	355,179	2	2	<RL	14	4	6,390	103	<RL	4	<RL	<RL	<RL	<RL	<RL	<RL
47	OH-C <sub>2</sub> F <sub>3</sub> H-(C <sub>2</sub> F <sub>4</sub> O) <sub>3</sub> -CF <sub>2</sub> COOH	3c	100,941	161	142	6	72	63	1,420	6,330	<RL	191	28	1	<RL	<RL	<RL	<RL
48	Polyfluoroether alcohol	3c	68,299	1,110	1,160	8	621	295	2,050	5,180	<RL	505	39	55	30	<RL	<RL	<RL
34	HPFPECA(1,1)	3a	110,213	95	99	13	61	220	6,530	20,700	<RL	176	84	<RL	2	<RL	<RL	<RL
<b>Reporting Class Sum</b>				5,238	4,374	39	2,691	2,234	104,457	67,068	3	8,978	734	181	43	0	0	0



**Table 7. Scaled Peak Area of Samples Calculated as the Ratio of Sample Peak Area to Reporting Limit Peak Area for PVDF Sulfonate Compounds (Report Class 4) Determined with Non-targeted Analysis (continued next page).**

Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area PVDF Sulfonate Compounds														
				INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
49	H-(C2F2H2)n-C2H2-SO3H (n=5)	4a	177,881	<RL	<RL	50	12	556	54,100	52,100	<RL	41	298	<RL	1	<RL	<RL	<RL
50	H-(C2F2H2)n-C2H2-SO3H (n=6)	4a	173,179	<RL	<RL	43	10	499	50,900	46,100	<RL	34	252	<RL	<RL	<RL	<RL	<RL
51	H-(C2F2H2)n-C2H2-SO3H (n=4)	4a	144,350	<RL	<RL	55	12	441	50,400	42,100	<RL	42	241	<RL	1	<RL	<RL	<RL
52	H-(C2F2H2)n-C2H2-SO3H (n=7)	4a	58,681	<RL	<RL	66	19	798	110,000	78,400	<RL	42	361	<RL	2	<RL	<RL	<RL
53	H-(C2F2H2)n-C2H2-SO3H (n=3)	4a	256,655	<RL	<RL	16	3	103	10,900	11,400	<RL	13	57	<RL	<RL	<RL	<RL	<RL
54	H-(C2F2H2)n-C2H2-SO3H (n=2)	4a	117,853	<RL	<RL	19	5	107	22,400	9,440	<RL	38	83	<RL	1	<RL	<RL	<RL
55	H-(C2F2H2)n-C2H2-SO3H (n=8)	4a	162,530	1	1	5	2	62	10,300	6,880	<RL	2	25	<RL	<RL	<RL	<RL	<RL
56	H-(C2F2H2)n-C2H2-SO3H (n=9)	4a	99,469	<RL	<RL	<RL	<RL	10	2,870	1,510	<RL	<RL	5	<RL	<RL	<RL	<RL	<RL
57	H-(C2F2H2)n-SO3H (n=5)	4b	250,580	11	11	58	33	701	66,000	61,800	<RL	182	186	<RL	2	<RL	<RL	<RL
58	H-(C2F2H2)n-SO3H (n=4)	4b	363,518	3	4	29	13	327	27,900	24,900	<RL	128	87	<RL	1	<RL	<RL	<RL
59	H-(C2F2H2)n-SO3H (n=6)	4b	316,686	4	3	27	10	315	28,300	29,400	<RL	57	82	<RL	<RL	<RL	<RL	<RL
60	H-(C2F2H2)n-SO3H (n=3)	4b	190,155	2	3	32	14	246	32,800	17,800	<RL	586	86	2	2	<RL	<RL	<RL
61	H-(C2F2H2)n-SO3H (n=7)	4b	212,635	2	2	18	5	215	20,400	20,400	<RL	42	60	<RL	<RL	<RL	<RL	<RL
62	H-(C2F2H2)n-SO3H (n=8)	4b	273,656	<RL	<RL	3	<RL	38	5,300	3,870	<RL	8	12	<RL	<RL	<RL	<RL	<RL
63	H-(C2F2H2)n-C3F6-SO3H (n=3)	4c	222,071	7	7	23	13	231	21,800	22,000	<RL	67	70	<RL	1	<RL	<RL	<RL
64	H-(C2F2H2)n-C3F6-SO3H (n=2)	4c	161,246	8	8	33	17	320	30,100	27,900	<RL	205	102	<RL	2	<RL	<RL	<RL
65	H-(C2F2H2)n-C3F6-O3SH (n=4)	4c	225,116	4	4	12	6	128	13,200	12,200	<RL	29	35	<RL	<RL	<RL	<RL	<RL
66	H-(C2F2H2)n-C3F6-SO3H (n=1)	4c	176,598	3	3	23	8	206	10,700	15,300	<RL	240	61	<RL	<RL	<RL	<RL	<RL
67	H-(C2F2H2)n-C3F6-SO3H (n=5)	4c	135,130	1	<RL	5	2	56	6,030	6,780	<RL	13	14	<RL	<RL	<RL	<RL	<RL
68	H-(C2F2H2)n-C3F6-SO3H (n=6)	4c	201,474	<RL	3	<RL	2	9	952	1,290	<RL	3	2	<RL	<RL	<RL	<RL	<RL
69	(C2F2H2)n-SO3 (n=5)	4d	228,129	2	2	11	9	118	16,900	10,400	<RL	67	34	<RL	<RL	<RL	<RL	<RL
70	(C2F2H2)n-SO3 (n=6)	4d	181,139	8	7	12	11	139	18,700	12,200	<RL	68	45	<RL	<RL	<RL	<RL	<RL
71	(C2F2H2)n-SO3 (n=7)	4d	16,626	2	<RL	18	7	205	35,500	23,200	<RL	96	79	<RL	<RL	<RL	<RL	<RL
72	(C2F2H2)n-SO3 (n=4)	4d	51,234	<RL	<RL	7	5	84	10,400	10,700	<RL	77	20	<RL	<RL	<RL	<RL	<RL

				Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area PVDF Sulfonate Compounds														
Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
73	(C2F2H2)n-SO3 (n=8)	4d	33,637	<RL	<RL	2	<RL	10	6,990	4,370	<RL	7	16	<RL	<RL	<RL	<RL	<RL
74	(C2H2F2)n-C5H10-SO3 (n=3)	4e	149,231	<RL	<RL	4	2	35	11,200	5,390	<RL	8	24	<RL	<RL	<RL	<RL	<RL
75	(C2H2F2)n-C5H10-SO3 (n=2)	4e	119,574	<RL	<RL	3	1	40	7,350	5,800	<RL	7	13	<RL	<RL	<RL	<RL	<RL
76	(C2H2F2)n-C5H10-SO3 (n=4)	4e	88,543	<RL	<RL	3	2	27	8,950	4,740	<RL	5	20	<RL	<RL	<RL	<RL	<RL
77	(C2H2F2)n-C5H10-SO3 (n=1)	4e	166,592	<RL	<RL	4	<RL	34	4,650	4,440	<RL	5	30	<RL	<RL	<RL	<RL	<RL
78	(C2H2F2)n-C5H10-SO3 (n=5)	4e	137,388	<RL	<RL	2	1	29	5,550	3,490	<RL	4	16	<RL	<RL	<RL	<RL	<RL
79	(C2H2F2)n-C5H10-SO3 (n=6)	4e	75,834	<RL	<RL	<RL	1	16	4,940	2,410	<RL	<RL	10	<RL	<RL	<RL	<RL	<RL
80	(C2H2F2)n-C5H10-SO3 (n=7)	4e	71,141	<RL	<RL	<RL	<RL	4	1,310	1,160	<RL	<RL	2	<RL	<RL	<RL	<RL	<RL
81	(C2H2F2)n-C3H6-SO3 (n=3)	4f	85,325	<RL	<RL	<RL	<RL	5	1,910	1,200	<RL	2	1	<RL	<RL	<RL	<RL	<RL
82	(C2H2F2)n-C3H6-SO3 (n=4)	4f	76,598	<RL	<RL	<RL	<RL	7	1,930	564	<RL	2	2	<RL	<RL	<RL	<RL	<RL
83	(C2H2F2)n-C3H6-SO3 (n=6)	4f	29,710	<RL	<RL	<RL	<RL	14	4,750	2,600	<RL	<RL	2	<RL	<RL	<RL	<RL	<RL
84	(C2H2F2)n-C3H6-SO3 (n=5)	4f	19,292	<RL	<RL	3	<RL	22	2,510	3,470	<RL	2	12	<RL	<RL	<RL	<RL	<RL
85	(C2H2F2)n-C3H6-SO3 (n=7)	4f	30,025	<RL	<RL	<RL	<RL	4	1,190	769	<RL	<RL	2	<RL	<RL	<RL	<RL	<RL
86	H(C2H2F2)n-C3H6-SO3H (n=3)	4g	104,068	<RL	<RL	3	<RL	36	2,900	3,540	<RL	4	3	3	<RL	<RL	<RL	<RL
87	H(C2H2F2)n-C3H6-SO3H (n=2)	4g	47,057	<RL	<RL	<RL	1	4	7,760	4,340	<RL	7	3	<RL	<RL	<RL	<RL	<RL
88	H(C2H2F2)n-C3H6-SO3H (n=6)	4g	60,310	<RL	<RL	<RL	<RL	5	1,490	653	<RL	<RL	3	<RL	<RL	<RL	<RL	<RL
89	H(C2H2F2)n-C3H6-SO3H (n=7)	4g	121,172	2	2	<RL	1	4	729	471	<RL	<RL	1	<RL	<RL	<RL	<RL	<RL
49	H-(C2F2H2)n-C2H2-SO3H (n=5)	4a	177,881	<RL	<RL	50	12	556	54,100	52,100	<RL	41	298	<RL	1	<RL	<RL	<RL
50	H-(C2F2H2)n-C2H2-SO3H (n=6)	4a	173,179	<RL	<RL	43	10	499	50,900	46,100	<RL	34	252	<RL	<RL	<RL	<RL	<RL
51	H-(C2F2H2)n-C2H2-SO3H (n=4)	4a	144,350	<RL	<RL	55	12	441	50,400	42,100	<RL	42	241	<RL	1	<RL	<RL	<RL
52	H-(C2F2H2)n-C2H2-SO3H (n=7)	4a	58,681	<RL	<RL	66	19	798	110,000	78,400	<RL	42	361	<RL	2	<RL	<RL	<RL
53	H-(C2F2H2)n-C2H2-SO3H (n=3)	4a	256,655	<RL	<RL	16	3	103	10,900	11,400	<RL	13	57	<RL	<RL	<RL	<RL	<RL
54	H-(C2F2H2)n-C2H2-SO3H (n=2)	4a	117,853	<RL	<RL	19	5	107	22,400	9,440	<RL	38	83	<RL	1	<RL	<RL	<RL
<b>Reporting Class Sum</b>				61	60	586	227	6,209	732,961	597,477	0	2,134	2,458	5	14	0	0	0

**Table 8. Scaled Sample Peak Area Calculated as the Ratio of Sample Peak Area to Reporting Limit Peak Area for PVDF Sulfate Compounds (Report Class 5) Determined with Non-targeted Analysis (continued next page).**

				Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area PVDF Sulfate Compounds														
Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
90	(C2F2H2)n-SO4 (n=4)	5a	142,466	<RL	<RL	12	8	147	21,100	13,500	<RL	59	27	<RL	<RL	<RL	<RL	<RL
91	(C2F2H2)n-SO4 (n=6)	5a	138,774	<RL	<RL	14	6	137	18,800	13,000	<RL	49	40	<RL	<RL	<RL	<RL	<RL
92	(C2F2H2)n-SO4 (n=5)	5a	45,941	<RL	<RL	18	11	114	24,900	10,900	<RL	31	26	<RL	<RL	<RL	<RL	<RL
93	(C2F2H2)n-SO4 (n=3)	5a	81,887	<RL	<RL	5	2	50	6,940	5,720	<RL	2	2	<RL	<RL	<RL	<RL	<RL
94	H-(C2F2H2)n-SO4H (n=4)	5b	506,841	<RL	<RL	111	23	1,100	60,000	62,000	<RL	138	207	<RL	<RL	<RL	<RL	<RL
95	H-(C2F2H2)n-SO4H (n=5)	5b	285,639	<RL	<RL	166	34	1,620	93,200	104,000	<RL	138	309	<RL	<RL	<RL	<RL	<RL
96	H-(C2F2H2)n-SO4H (n=6)	5b	615,542	<RL	<RL	52	8	512	28,500	39,200	<RL	50	95	<RL	<RL	<RL	<RL	<RL
97	H-(C2F2H2)n-SO4H (n=3)	5b	126,023	1	2	202	44	1,760	105,000	94,300	<RL	941	343	<RL	1	<RL	<RL	<RL
98	H-(C2F2H2)n-SO4H (n=2)	5b	55,998	33	43	498	131	2,650	184,000	109,000	23	15,900	778	61	15	<RL	<RL	<RL
99	H-(C2F2H2)n-SO4H (n=7)	5b	411,639	<RL	<RL	20	3	192	11,800	17,000	<RL	20	32	<RL	<RL	<RL	<RL	<RL
100	H-(C2F2H2)n-SO4H (n=8)	5b	115,580	<RL	<RL	9	2	75	5,700	8,130	<RL	16	13	1	<RL	<RL	<RL	<RL
101	H-(C2F2H2)n-C3F6-SO4H (n=2)	5c	187,417	1	1	25	11	341	30,300	21,500	<RL	111	96	<RL	<RL	<RL	<RL	<RL
102	H-(C2F2H2)n-C3F6-SO4H (n=3)	5c	156,782	1	1	32	10	423	30,900	34,300	<RL	91	123	<RL	<RL	<RL	<RL	<RL
103	H-(C2F2H2)n-C3F6-SO4H (n=1)	5c	151,216	2	<RL	45	20	562	32,500	28,600	<RL	4	165	1	<RL	<RL	<RL	<RL
104	H-(C2F2H2)n-C3F6-SO4H (n=4)	5c	128,045	<RL	<RL	15	4	194	14,000	18,000	<RL	34	49	<RL	<RL	<RL	<RL	<RL
105	H-(C2F2H2)n-C3F6-SO4H (n=5)	5c	142,463	<RL	2	5	1	59	4,410	6,450	<RL	9	13	<RL	<RL	<RL	<RL	<RL
106	H-(C2F2H2)n-C3F6-SO4H (n=6)	5c	88,106	<RL	<RL	2	<RL	24	1,490	3,180	<RL	3	4	<RL	<RL	<RL	<RL	<RL
107	(C2H2F2)n-C5H10-SO4 (n=3)	5d	141,405	<RL	<RL	7	3	64	18,200	7,660	<RL	18	48	<RL	<RL	<RL	<RL	<RL
108	(C2H2F2)n-C5H10-SO4 (n=5)	5d	153,128	<RL	<RL	10	3	109	8,160	13,100	<RL	19	48	<RL	<RL	<RL	<RL	<RL
109	(C2H2F2)n-C5H10-SO4 (n=4)	5d	70,614	<RL	<RL	3	1	24	6,460	3,790	<RL	8	18	<RL	<RL	<RL	<RL	<RL
110	(C2H2F2)n-C5H10-SO4 (n=2)	5d	69,548	<RL	<RL	<RL	<RL	3	1,380	20	<RL	<RL	<RL	<RL	<RL	<RL	<RL	<RL

				Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area PVDF Sulfate Compounds														
Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
111	(C2H2F2)n-C7H12-SO4 (n=3)	5e	85,115	<RL	<RL	<RL	<RL	9	2,270	1,520	<RL	2	2	<RL	<RL	<RL	<RL	<RL
112	(C2H2F2)n-C7H12-SO4 (n=4)	5e	32,561	<RL	<RL	<RL	<RL	14	1,990	1,270	<RL	2	5	<RL	<RL	<RL	<RL	<RL
113	(C2H2F2)n-C7H12-SO4 (n=5)	5e	49,837	<RL	<RL	<RL	<RL	5	1,080	520	<RL	<RL	3	<RL	<RL	<RL	<RL	<RL
114	(C2H2F2)n-C7H12-SO4 (n=6)	5e	27,563	<RL	<RL	<RL	<RL	9	1,210	509	<RL	<RL	3	<RL	<RL	<RL	<RL	<RL
115	H(C2H2F2)n-SO5H (n=4, monoether)	5f	88,591	<RL	<RL	9	1	46	3,000	6,530	<RL	9	5	<RL	<RL	<RL	<RL	<RL
116	H(C2H2F2)n-SO5H (n=5, monoether)	5f	69,686	<RL	<RL	8	1	54	2,320	4,490	<RL	8	<RL	<RL	<RL	<RL	<RL	<RL
117	H(C2H2F2)n-SO5H (n=6, monoether)	5f	29,603	<RL	<RL	1	1	39	4,250	4,630	<RL	13	1	<RL	<RL	<RL	<RL	<RL
118	H(C2H2F2)n-SO5H (n=8, monoether)	5f	22,735	<RL	<RL	7	<RL	33	2,680	3,950	<RL	11	8	<RL	<RL	<RL	<RL	<RL
119	H(C2H2F2)n-SO5H (n=7, monoether)	5f	24,136	<RL	<RL	5	<RL	14	1,920	1,890	<RL	5	3	<RL	<RL	<RL	<RL	<RL
120	H(C2H2F2)n-C2H2O-SO4H (n=5)	5g	52,567	<RL	<RL	63	<RL	79	682	10,000	<RL	4	3	<RL	<RL	<RL	<RL	<RL
121	H(C2H2F2)n-C2H2O-SO4H (n=6)	5g	60,691	<RL	<RL	10	<RL	23	994	3,790	<RL	9	1	<RL	<RL	<RL	<RL	<RL
122	H(C2H2F2)n-C2H2O-SO4H (n=7)	5g	53,046	<RL	<RL	<RL	<RL	19	836	2,970	<RL	5	2	<RL	<RL	<RL	<RL	<RL
123	H(C2H2F2)n-C2H2O-SO4H (n=4)	5g	92,010	<RL	<RL	<RL	<RL	3	1,590	433	<RL	1	<RL	<RL	<RL	<RL	<RL	<RL
124	H(C2H2F2)n-C2H2O-SO4H (n=8)	5g	118,124	<RL	<RL	<RL	<RL	12	716	1,120	<RL	4	<RL	<RL	<RL	<RL	<RL	<RL
125	H(C2H2F2)n-C2H4O-SO4H (n=7)	5h	66,410	<RL	<RL	2	<RL	39	4,300	4,380	<RL	18	10	<RL	<RL	<RL	<RL	<RL
126	H(C2H2F2)n-C2H4O-SO4H (n=5)	5h	68,811	<RL	<RL	2	<RL	16	1,100	1,910	<RL	1	<RL	<RL	<RL	<RL	<RL	<RL
127	H(C2H2F2)n-C2H4O-SO4H (n=6)	5h	46,419	<RL	<RL	1	<RL	20	1,510	2,510	<RL	2	1	<RL	<RL	<RL	<RL	<RL
128	H(C2H2F2)n-C2H4O-SO4H (n=4)	5h	78,226	<RL	<RL	<RL	<RL	6	677	959	<RL	2	<RL	<RL	<RL	<RL	<RL	<RL
129	H(C2H2F2)n-C2H4O-SO4H (n=8)	5h	49,953	3	3	<RL	2	7	714	928	<RL	3	1	<RL	<RL	<RL	<RL	<RL
<b>Reporting Class Sum</b>				42	52	1,358	330	10,605	741,579	667,659	23	17,738	2,482	63	17	0	0	0

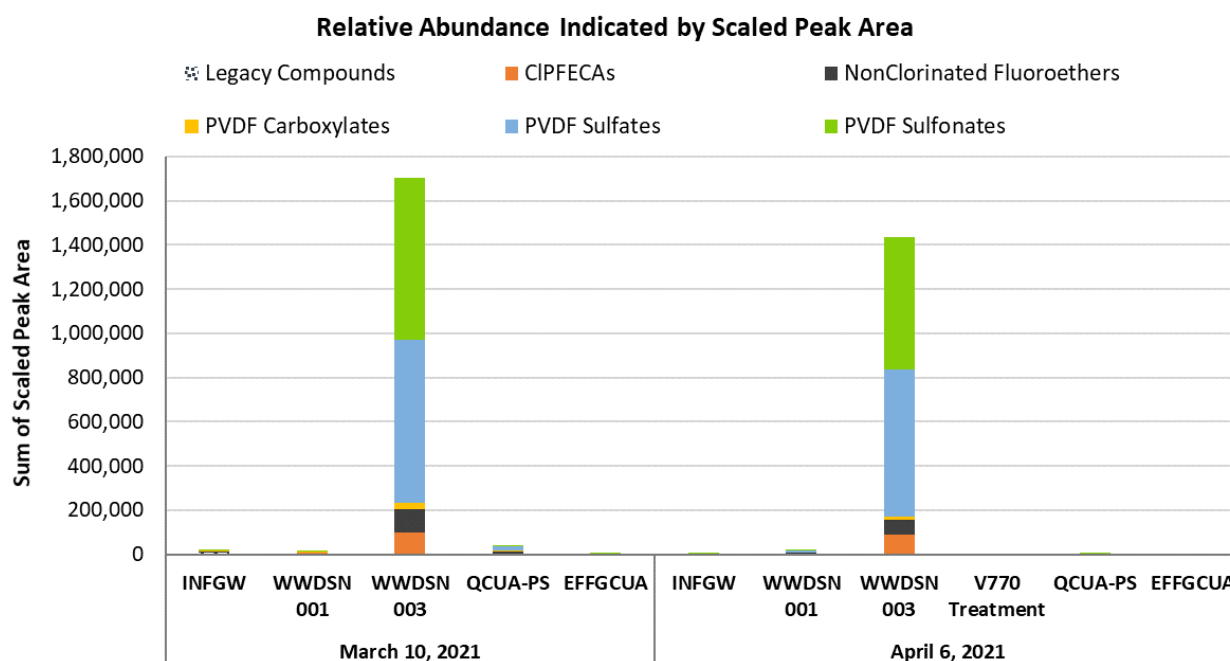
**Table 9. Scaled Sample Peak Area Calculated as the Ratio of Sample Peak Area to Reporting Limit Peak Area for PVDF Carboxylate Compounds (Report Class 6) Determined with Non-targeted Analysis.**

Chem Ref #	Compound	Report Class	Reporting Limit Peak Area	Ratio of Sample Peak Area to Analyte Reporting Limit Peak Area PVDF Carboxylate Compounds														
				INF GW 01	WW DUP 01	INF GW 02	WWD SN 001 01	WWD SN 001 02	WWD SN 003 01	WWD SN 003 02	V770 Treat 02	GCUA PS 01	GCUA-PS 02	EFF GCUA 01	EFF GCUA 02	WW FB 01	WW FB 02	TB 02
130	H-(C2F2H2)n-C3F6-COOH (n=1, oxidized HFPO+PVDF)	6a	80,935	30	33	3	17	23	5,310	2,220	<RL	576	2	5	<RL	<RL	<RL	<RL
131	H-(C2F2H2)n-C3F6-COOH (n=3)	6a	28,035	11	11	<RL	5	16	2,270	1,310	<RL	20	4	<RL	<RL	<RL	<RL	<RL
132	H-(C2F2H2)n-C3F6-COOH (n=2)	6a	53,452	4	4	<RL	<RL	5	902	12	<RL	21	<RL	<RL	<RL	<RL	<RL	<RL
133	H-(C2F2H2)n-C3F6-COOH (n=4)	6a	27,812	7	6	<RL	4	10	1,440	1,080	<RL	8	4	<RL	<RL	<RL	<RL	<RL
134	H-(C2F2H2)n-CF2-COOH (n=4)	6b	521,971	241	255	4	132	89	6,110	3,010	<RL	116	64	1	7	<RL	<RL	<RL
135	H-(C2F2H2)n-CF2-COOH (n=2)	6b	649,395	99	101	7	39	50	1,900	456	8	3,880	45	64	8	<RL	<RL	<RL
136	H-(C2F2H2)n-CF2-COOH (n=6)	6b	37,012	386	305	3	166	131	5,940	2,670	<RL	152	65	<RL	6	<RL	<RL	<RL
137	H-(C2F2H2)n-CF2-COOH (n=5)	6b	52,964	543	540	<RL	287	116	988	644	<RL	46	20	<RL	3	<RL	<RL	<RL
138	H-(C2F2H2)n-CF2-COOH (n=3)	6b	54,283	304	335	<RL	164	71	198	101	<RL	79	12	8	22	<RL	<RL	<RL
139	H-(C2F2H2)n-COOH (n=4)	6c	62,694	<RL	<RL	1	<RL	5	930	932	<RL	5	1	1	<RL	<RL	<RL	<RL
140	H-(C2F2H2)n-COOH (n=5)	6c	101,823	2	3	<RL	292	3	126	4	<RL	1	<RL	3	<RL	<RL	<RL	<RL
141	H-(C2F2H2)n-COOH (n=6)	6c	26,445	7	7	<RL	675	<RL	156	<RL	<RL	3	<RL	1	<RL	<RL	<RL	<RL
130	H-(C2F2H2)n-C3F6-COOH (n=1, oxidized HFPO+PVDF)	6a	80,935	30	33	3	17	23	5,310	2,220	<RL	576	2	5	<RL	<RL	<RL	<RL
131	H-(C2F2H2)n-C3F6-COOH (n=3)	6a	28,035	11	11	<RL	5	16	2,270	1,310	<RL	20	4	<RL	<RL	<RL	<RL	<RL
132	H-(C2F2H2)n-C3F6-COOH (n=2)	6a	53,452	4	4	<RL	<RL	5	902	12	<RL	21	<RL	<RL	<RL	<RL	<RL	<RL
133	H-(C2F2H2)n-C3F6-COOH (n=4)	6a	27,812	7	6	<RL	4	10	1,440	1,080	<RL	8	4	<RL	<RL	<RL	<RL	<RL
<b>Reporting Class Sum</b>				1,634	1,599	17	1,781	519	26,270	12,439	8	4,906	217	82	45	0	0	0

Sample results are briefly summarized in Figures 5 through 7 illustrating PFAS emissions at locations within the facility and between the two sampling events. PFAS emissions may differ between samplings depending on what processing lines were operating at the time of collection. The CIPFPECA process was “in service” during sampling 2. PFAS are characterized as the sum of Scaled Peak Area for each class of compounds. These summed values are available in Tables 4-9.

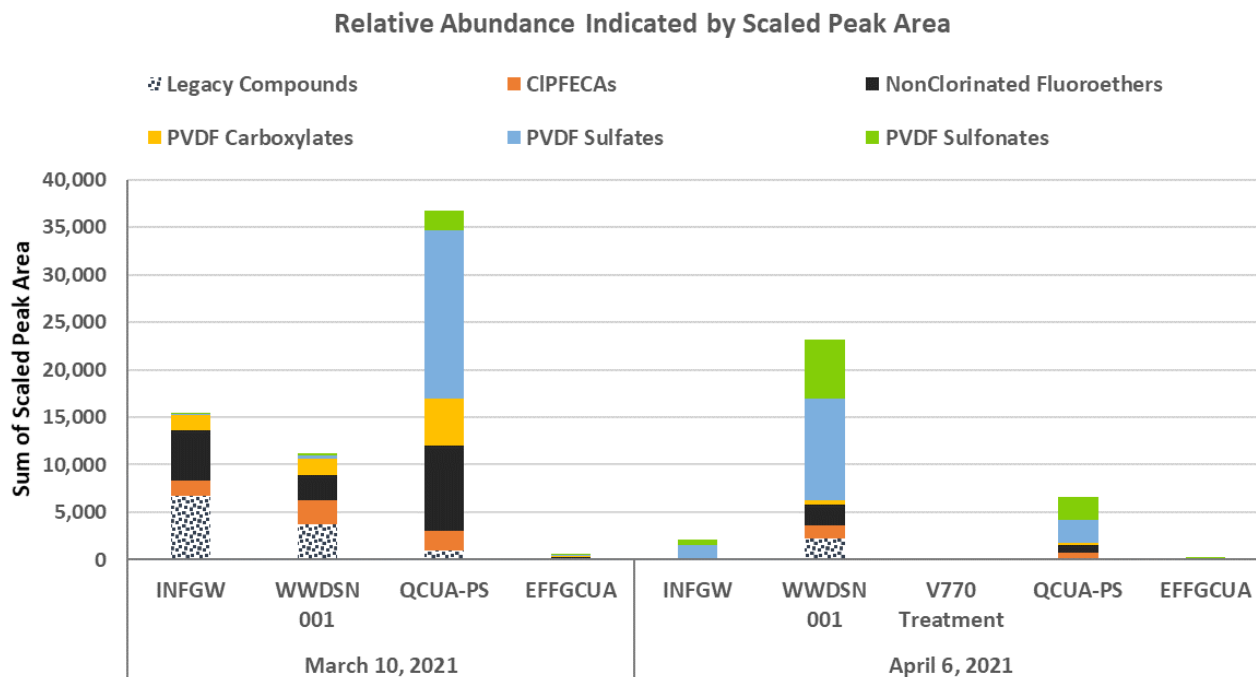
Figure 5 shows the total PFAS emissions at all sampling locations in both sampling events. The total PFAS emissions was far greater in the waste discharge line represented by WWDSN003 than at any other location in the facility. WWDSN003 is sampled before the waste stream is sent through treatment. The post-treatment waste concentrations that are sent to GCUA are represented by V770. The PVDF sulfates and sulfonates make up the majority of the PFAS emissions in the waste stream prior to treatment but all compound classes were present. Results were relatively similar between the sampling events at this location.

**Figure 5. Relative abundance of compound classes at sampling locations determined by the by the Scaled Peak Areas summed by compound class.**



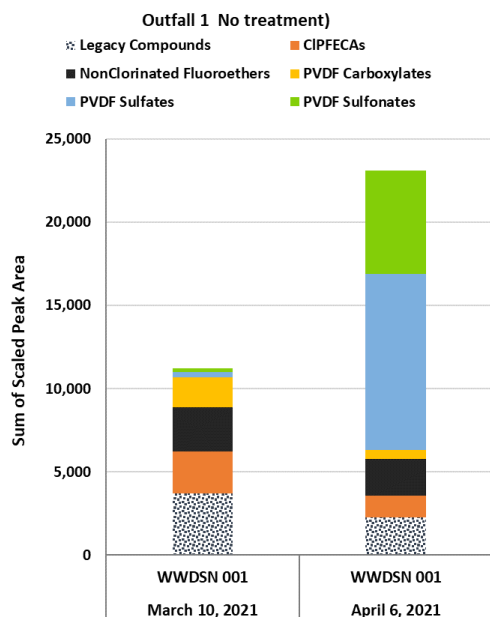
In order to better visualize the relative differences in emissions among the other sampling locations with less abundance, Figure 6 also shows the total PFAS emissions at locations in the Solvay plant during the two sampling events but with WWDSN003 removed. As determined in targeted analysis, the groundwater inflow (INFGW) was contaminated with a number of legacy compounds as well as with Cl-PFPECA, non-chlorinated fluoroether, and PVDF carboxylate groups. There were relatively little to no sulfonates or sulfates in sampling 1, although these compounds were more prevalent in sampling 2. PFAS are detectable in WWDSN001 outfall that discharges to surface water and appears to be circulated from groundwater and/or other sources within the facility.

**Figure 6. Relative abundance of compound classes at sampling locations determined by the by the Scaled Peak Areas summed by compound class. The graphic excludes sampling location WWDSN-003 to allow comparison of other locations.**

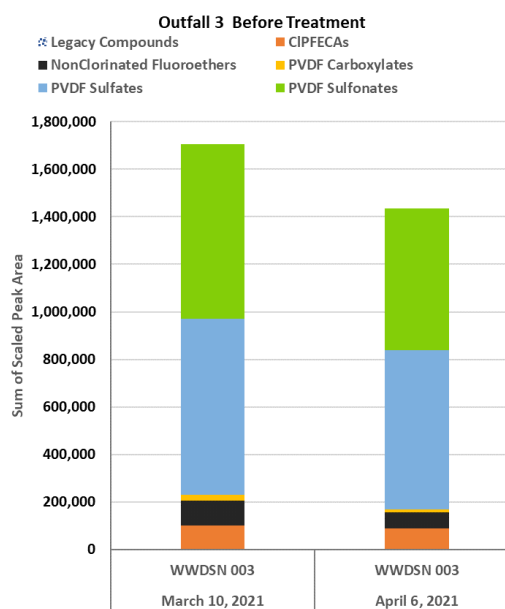


**Figure 7. Relative abundance of compound classes at WWDSN 001 (A) discharged to surface water and WWDSN003 (B) prior to process wastewater treatment within the Solvay facility as determined by the by the Scaled Peak Areas summed by compound class. Note differences in y-axis scales between locations.**

A)



B)



WWDSN001 releases discharge directly to the Delaware River but discharge from WWDSN003 is treated before it is sent to GCUA. This waste stream was sampled post-treatment during sampling 2 at an access port installed by Solvay. Treatment appears to be very effective as almost no PFAS of any class were sent to GCUA from the treated process waste stream (Figure 6 and Tables 4-9).

Figure 7 shows the abundance of compound classes at each of the WDSN outfalls in each of the samplings. (Note the differences in scales between A) and B) to allow comparison of compounds). Sampling event 2 on April 6 when the CIPFECA process was “in service” leads to only small increases in the CIPFECA abundance between samplings. However, the PVDF based PFAS was constantly released at WWDN003 and increased significantly at WWDSN 001 in sampling 2.

### Summary of Quality Control Measures

With NTA, there are few quality control analytical performance measures or criteria available to assess retention from field collection, shipping, storage, recovery through laboratory preparation, purification processes, or the accuracy and precision of the analytical methods used. However, field and laboratory quality control samples as well as internal standards injected by the laboratory into processed samples allowed for some assessment of the reliability and repeatability of the NTA results.

A total of 12 samples were collected in the two separate sampling events (March 10 and April 6, 2021). Each sampling was processed in separate batches. A field duplicate was collected during sampling 1. A field blank and 2 blanks spiked with known concentrations of legacy compounds prepared by the ORD laboratory were transported to the field in each sample event. An unopened trip blank was transported to the field during sampling 2. Additional QC measures were applied in the laboratory. Laboratory processing included one method blank with each batch. In addition, the samples contained calibration standards for the 9 legacy compounds injected at varying amounts during targeted analysis. The laboratory also injected 11 internal standards into the samples and blanks in constant amounts to assess potential losses during the analytical process. All QC measures in the following analyses are applied to the peak areas of the unknown and QC samples.

**FIELD DUPLICATE.** A field duplicate (WWDUP-01) was obtained at the groundwater inflow location paired with sample INFGW-01 during the March 10 sampling. Sample results for 141 analytes are provided in Tables 3-8. The relative percent difference (RPD) of the raw peak area of each analyte was computed to indicate method precision according to equation 3. The goal for NTA analysis is  $RPD < 50\%$ .

$$Eq\ 3. \text{ Relative Percent Difference (RPD, \%)} = \left( \frac{ABS(\text{Sample 1} - \text{Sample 2})}{((\text{Sample 1} + \text{Sample 2})/2)} \right) \times 100\%$$

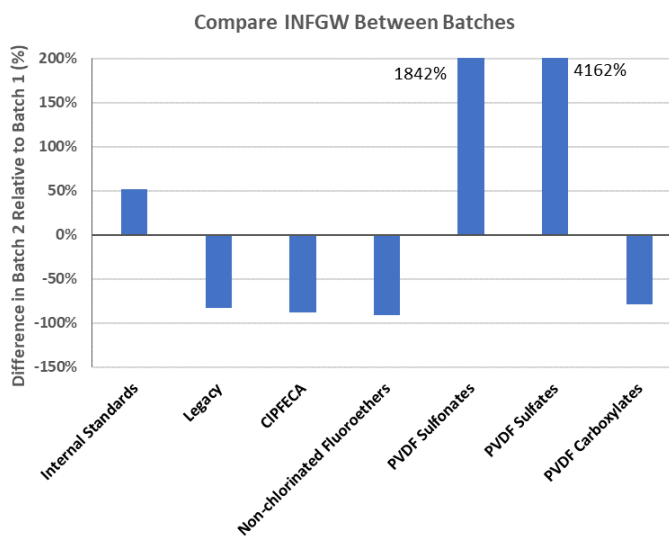
Excellent precision results for peak areas were observed in the field duplicate pair collected at the same location and time. None of the 141 analytes exceeded the project goal and just eight exceeded an RPD of 10%. The overall average RPD of analytes was 4.6%. The average RPD of the injected internal standards was 1.1%. This high precision in the duplicate pair was also observed in targeted analysis<sup>4</sup>.

One expectation of the sampling plan was that the chemistry of effluent locations could vary between sampling dates due to differences in operations within the plant. In contrast, the groundwater inflow where the duplicates were collected would not be expected to change significantly in the nearly 1-month period between samplings. Similar concentrations of legacy compounds were observed between samplings at this location in targeted analysis<sup>4</sup>. However, NTA analysis found significant differences in the peak areas of analytes in the sample as indicated in Tables 4-9 and Figure 6. Many of the analytes, including the legacy



compounds, were significantly lower in batch 2, while others were significantly higher. The difference in peak areas between batches is further illustrated by the ratio of the two in Figure 8. While site-specific conditions may suggest that relatively rapid changes in groundwater inflow chemistry could occur at this location, it is possible that the differences between batches at this location could indicate some analytical bias was introduced. Therefore, where appropriate, this QC discussion includes assessment of any systematic patterns in QC metrics between samplings that could indicate analytical bias.

**Figure 8. Comparison of peak areas in groundwater samples collected at INFGW between batches. The difference between batches is shown as shown as the percent difference in peak area in batch 2 relative to peak area in batch 1. The values shown are the average of all analytes in the compound class.**

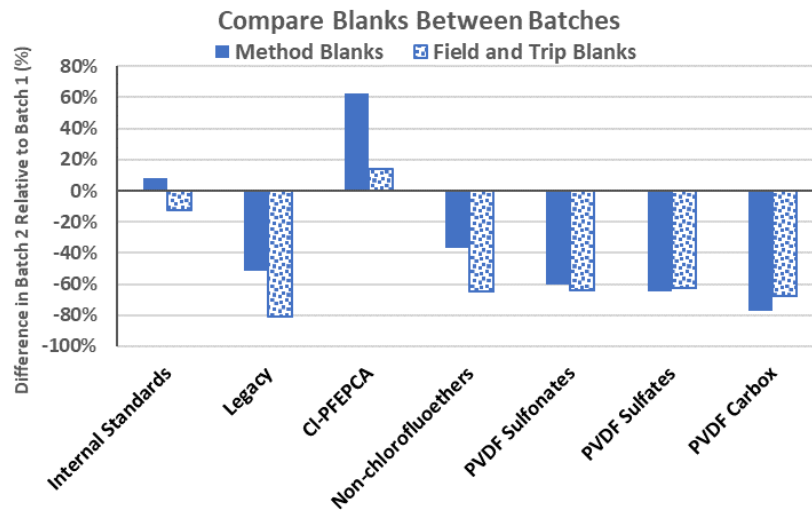


**LABORATORY BLANKS.** Raw peak areas were observed in method blanks (MB) below the “noise” level of the UPLC/MS instrument software. These peak areas were used to establish the reporting limit (RL) for each analyte as described earlier. The project quality goal for laboratory and field blanks is for the peak area to not exceed this “noise” threshold.

Neither of the methods blanks contained peak areas of any of the 141 PFAS compounds in abundance greater than RL. Comparing batches, the peak areas of all of the analyte classes except Cl-PFEPCA were significantly lower in the batch 2 methods blanks, indicating the second batch was somewhat “cleaner” with less processing noise than the first (Fig. 9). The average ratio of peak areas in batch 2 to batch 1 was 57% while the internal standards in the methods blanks were similar between batches and varied by less than 10%.

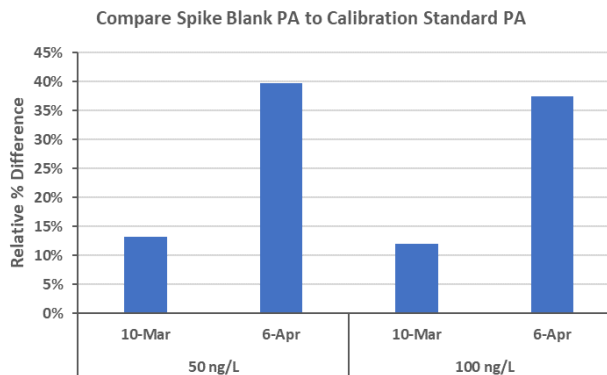
**FIELD and TRIP BLANKS.** Peak areas for 141 PFAS analytes in the 2 field blanks and the trip blank were generally less than the reporting limit (Tables 4-9). Just 3 of 423 total measurements exceeded RL. These results indicate no discernible contamination during field sampling. The lower peak areas in batch 2 laboratory blanks carried over to batch 2 field blanks, confirming that laboratory processing in batch 2 was generally “cleaner” than batch 1. The peak areas in blanks between samplings are compared in Figure 9. Note that the extent of batch differences for some compound classes at INFGW are consistent with those in the blanks while others are quite different.

**Figure 9. Comparison of peak areas in laboratory and field blanks between batches. The difference between batches is shown as the percent difference in peak area in batch 2 relative to peak area in batch 1. The values shown are the average of all analytes in the compound class.**



**SPIKE BLANKS.** One bottle spiked with 50 ng/L and 1 bottle spiked with 100 ng/L of the 9 legacy analytes quantitated with targeted analysis were prepared by ORD, sent to NJ DEP in the week prior to sampling, and were carried to the field in each sampling event. NTA results for the spiked blanks demonstrated that the peak areas determined during NTA were sensitive to known differences in the concentrations of the compounds injected into the samples. The peak areas of compounds in the spiked blanks were within 50% of the peak area of the relevant calibration standards in each of the 4 samples (Figure 10). Spiked blank peak areas were closest to the peak area of calibration standards in batch 1 when the calibration standards were added but were acceptable in both batches. As with the other blanks, the peak areas of the 50 ng/L and 100 ng/L spiked blanks were generally lower in batch 2 than batch 1, but by only 22% and 34% respectively.

**Figure 10. Average relative percent difference (RPF) of the peak area of legacy analytes in the spike blanks relative to the peak area in the calibration standards.**



**INTERNAL STANDARDS.** A known amount of 11 internal standards were added to all 27 of the samples, blanks and calibration standards during preparation for the non-targeted analysis. The peak area within each standard should be similar in the known and unknown samples unless there was loss in the laboratory analytical process. Internal standard characteristics and the peak areas measured in samples are provided in Appendix C.

The differences in peak area of individual samples from the grand average of all samples within each internal standards were calculated as an indicator of internal standard recovery. Recovery within  $\pm 50\%$  would be considered very good for NTA. Summarized results are provided in Table 10. Internal standards were reliably recovered across all 11 of the internal standards and all sample types. The difference among internal

standards averaged among all sample types for each IS ranged from -6.2% to +14.3%. Of the 297 individual comparisons, 12 (4%) were outside the range of  $\pm 50\%$ .

Recovery was very consistent among most of the internal standards, although recovery was especially variable within M7PFUnDA. We also note that there was greater variability in recovery among the methods blanks than other sample types, with several of the standards showing much higher peak areas than the group average, again associated with M7PFUnDA. In general, confidence in reported results is lower for the legacy compound PFUnDA than other analytes.

**Table 10. Percent difference in peak area of internal standard of individual samples relative to average peak area of all samples in the internal standard group.**

AVERAGE of Group	Percent Difference of Peak Area of Internal Standard to Average of Peak Area for Entire Sample Set										
	MPFBA	M5PFPeA	M5PFHxA	M4PFHpA	M8PFOA	M9PFNA	M6PFDA	M7PFUnDA	M3PFBS	M3PFHxS	M8PFOS
Cal Standard	-15.3%	1.9%	6.3%	10.2%	8.4%	8.4%	-12.5%	-26.3%	-22.9%	-1.2%	-10.8%
Spike Blanks	2.4%	-9.5%	3.3%	-0.8%	4.3%	8.1%	3.3%	10.4%	-10.3%	-3.1%	-1.7%
MB	0.0%	-13.2%	-1.9%	0.9%	10.2%	19.8%	44.0%	95.3%	-13.0%	-8.6%	6.0%
Field Blanks	7.9%	-16.7%	-0.4%	-4.9%	2.7%	-1.3%	-9.4%	-2.6%	-2.7%	6.9%	-1.4%
Samples	4.9%	8.6%	-3.8%	-3.7%	-8.0%	-9.9%	0.2%	-5.6%	17.7%	1.3%	5.3%
Average	0.0%	-5.8%	0.7%	0.3%	3.5%	5.0%	5.1%	14.3%	-6.2%	-0.9%	-0.5%

The averaged RPD of internal standards compared between repeated unknown and QC samples in Table 11. The averaged RPD of internal standards compared between repeated unknown and QC samples ranged from 2 to 12% and no internal standard/sample combination exceeded 50%. There were no identifiable trends in internal standard recovery across batches to indicate analytical bias. We note that the highest RPD occurred in M7PFUnDA in the groundwater inflow sample (INFGW), while the RPD of other standards were similar at this location.

**Table 11. Relative percent difference between batch 1 and 2 for internal standards in quality control and unknown samples.**

	QC				Samples				
	Method Blank	Field Blank	Spiked Blank Low	Spiked Blank High	INFGW	WWDSN001	GCUA-PS	WWDSN003	EFF-GCUA
MPFBA	15%	5%	12%	8%	4%	0%	12%	9%	1%
M5PFPeA	16%	22%	14%	18%	16%	10%	11%	9%	4%
M5PFHxA	11%	16%	7%	11%	8%	2%	7%	2%	1%
M4PFHpA	13%	16%	8%	9%	10%	1%	7%	6%	5%
M8PFOA	5%	7%	0%	0%	12%	17%	1%	1%	1%
M9PFNA	7%	4%	5%	4%	20%	15%	16%	6%	5%
M6PFDA	20%	12%	2%	4%	19%	5%	14%	0%	7%
M7PFUnDA	27%	16%	5%	1%	31%	4%	18%	3%	0%
M3PFBS	3%	1%	8%	2%	1%	5%	6%	3%	2%
M3PFHxS	4%	4%	3%	0%	6%	10%	5%	0%	0%
M8PFOS	4%	2%	0%	0%	0%	2%	17%	7%	1%
Average	11%	10%	6%	5%	12%	6%	10%	4%	2%

SUMMARY OF QC MEASURES. The NTA analysis reliably isolated compounds and determined the relative intensities across all unknown and quality control samples. Where those intensities could be correlated to peak areas at known concentrations, they compared favorably. Blanks were clean of contamination and there was no indication of significant contamination or other problems with analysis.

There were some differences between batches that was evident in the blank samples. Peak areas in blanks were lower in batch 2, indicating less analytical interference in this set of samples. The blanks establish the reporting limit for samples which in turn influenced the Scaled Peak Area reported in Tables 3-8. The differences between batches are blended in the statistical calculation and therefore there is relatively little impact on the reported results.

The internal standards showed very good consistency among sample types and between batches indicating good analytical recovery and consistency of analysis. There were no indications of analytical bias between batches within the expected variability in NTA analysis.

We have noted that the NTA results indicate some differences in the relative abundance of a limited number of legacy compounds collected in the two sampling events at the groundwater sampling location (INFGW) compared to findings from targeted analysis presented in NJDEP Report #10<sup>4</sup>. Our assessment of QC measures available with the NTA analysis identified no analytical biases or failures that may have contributed to those differences.

## Appendix A: Interpretation of Compound Identification Confidence

Each uniquely identified chemical feature is assigned a confidence score based on available information used to make the assignment and the quality of reference data available. We report a confidence score of 1 to 5, loosely based on the framework of Schymanski et al. *Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence* (doi: [10.1021/es5002105](https://doi.org/10.1021/es5002105)). The best score for each chemical is reported.

All compounds in this report met criteria for priority 1 and 2. There are no compounds with priority 3 or 4 reported.

The scoring criteria are described below:

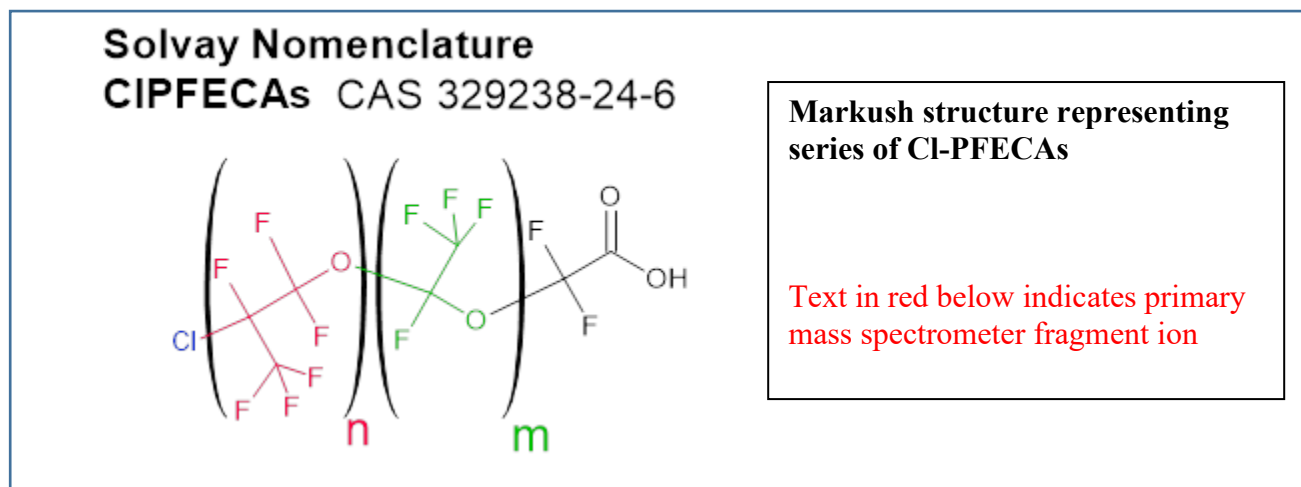
<b>Priority</b>
1 = confirmed PFAS chemical based on manual examination of fragmentation spectrum and/or computerized match against a reference spectrum
2 = likely PFAS based on formula generation, manually examined for feasibility
3 = probably PFAS-like compound on the basis of negative mass defect in > 0.85, < 0.05 range
4 = unlikely PFAS on the basis of available MS information OR duplicate PFAS ion generated as instrumental artefact (fragments, dimers, and/or adducts when parent can be observed)
<b>Confidence (based on Schymanski scale (DOI: 10.1021/es5002105))</b>
1 = Confirmed by comparison with reference chemical
2a = Likely structure based on computerized spectrum match
2b = Likely structure based on manual interpretation of MS/MS spectrum
3 = Tentative candidate or MS data insufficient for unequivocal identification beyond class (i.e. PFAS chemical)
4 = Formula level identification only (MS/MS unavailable)
5 = Exact mass level identification only (no predicted formula)

## Appendix B. Solvay and EPA nomenclature for Cl-PFECA Compounds

Solvay refers to the ClPFPECA compounds as monofunctional surfactants (MFS) with the generic structure shown in Figure B-1. The terminal Cl-C<sub>2</sub>F<sub>6</sub>O is treated as an additional “n” group with a Cl at the end. According to Solvay nomenclature the (n) is the propyl group and the (m) the ethyl group.

In previous data reports, EPA positionally switched the “m” and “n” in compound representations from those used by Solvay. To be consistent with Solvay nomenclature, this report uses Solvay conventions. The naming conventions used by Solvay and EPA for these chemicals are provided in Table B-1 To assist with comparison to data provided in earlier reports.

**Figure B-1. Representative Markush Structure for Solvay Cl-PFECAs**



**Table B-1. Molecular formula, name, and monoisotopic mass of chemicals.**

Formula	Solvay Name	EPA Name	M-H monoisotopic mass (g/mol)
C <sub>8</sub> H Cl F <sub>14</sub> O <sub>4</sub>	MFS-N2	Cl-PFECA 0,1	460.9267
C <sub>11</sub> H Cl F <sub>20</sub> O <sub>5</sub>	MFS-N3	Cl-PFECA 0,2	626.912
C <sub>14</sub> H Cl F <sub>26</sub> O <sub>6</sub>	MFS-M4	Cl-PFECA 0,3	792.8974
C <sub>17</sub> H Cl F <sub>32</sub> O <sub>7</sub>	MFS-N5	Cl-PFECA 0,4	958.8827
C <sub>8</sub> H Cl F <sub>16</sub> O <sub>3</sub>	MFS-M3	Cl-PFECA 1,1	576.9152
C <sub>13</sub> H Cl F <sub>24</sub> O <sub>6</sub>	MFS-M4	Cl-PFECA 1,2	742.9006

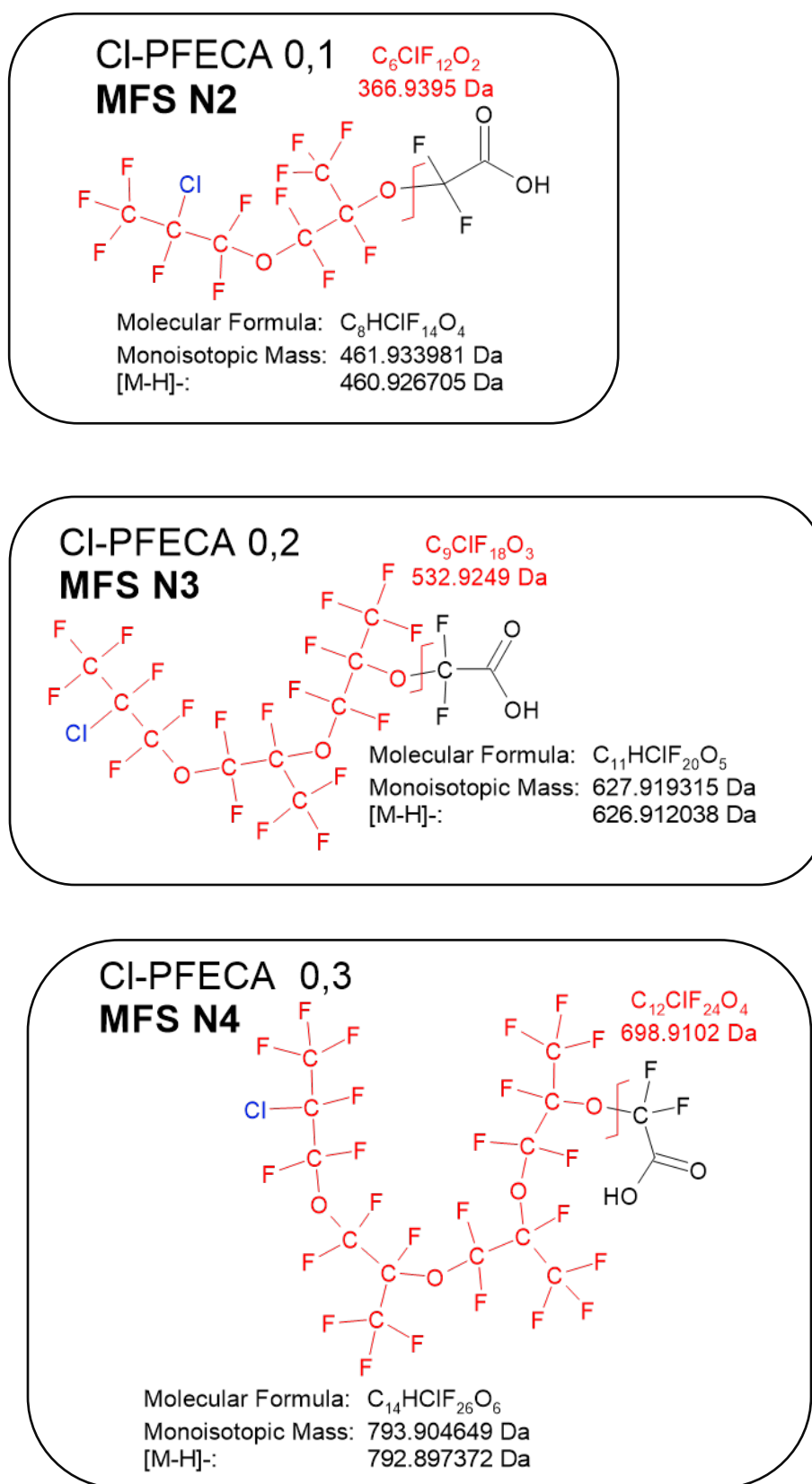
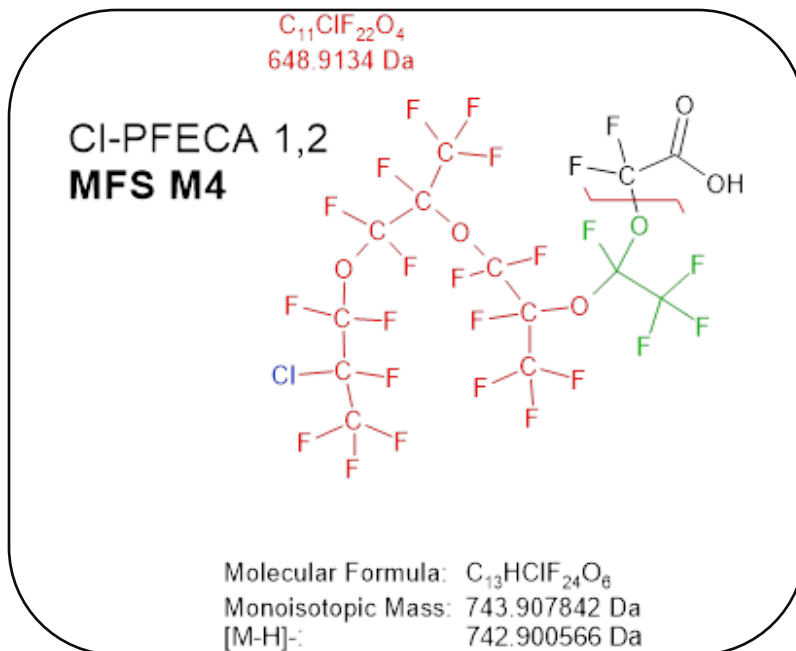
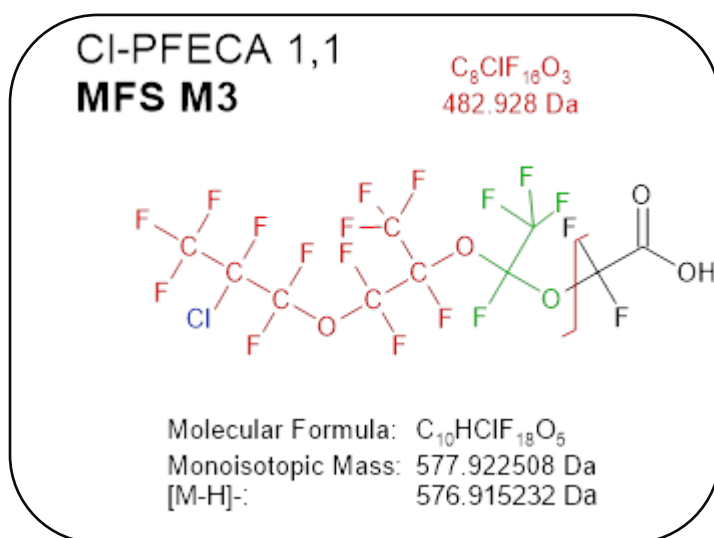
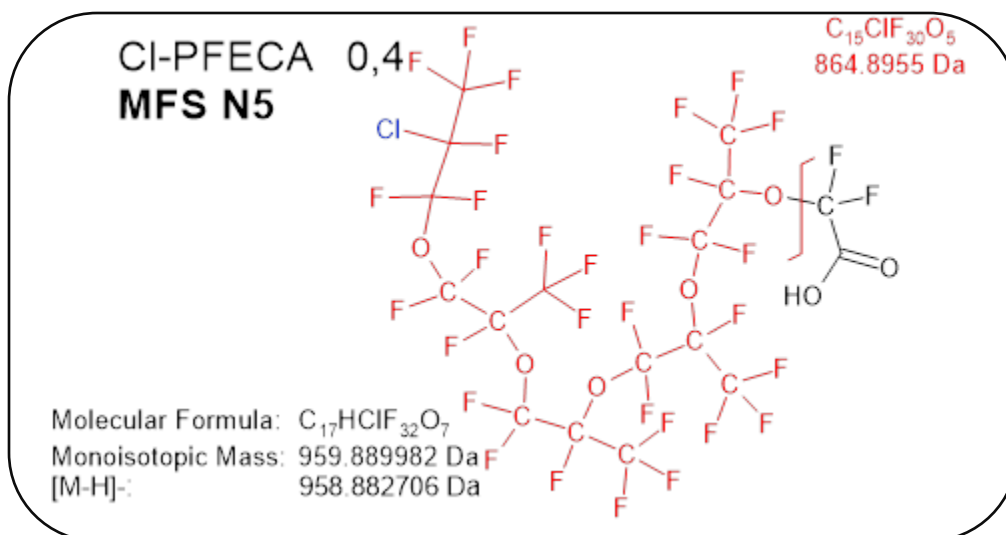
**Figure B-2. Individual structures, names and characteristics of representative CI-PFECA. (n=6) shown.**

Figure B-2. Continued





## Appendix C. Internal Standards Used in PFAS NTA Analysis

Table C.1. Internal Standards Characteristics and Peak Area

Internal Standard	Formula	Monoisotopic Mass (g/mol)	RT
MPFBA	[13C4]HF7O2	217.9999	1.032
M5PFPeA	[13C]5HF9O2	269.0000	2.333
M5PFHxA	[13C]5CHF11O2	318.9968	3.690
M4PFHpA	[13C]4C3HF13O2	367.9903	4.755
M8PFOA	[13C]8HF15O2	422.0005	5.634
M9PFNA	[13C]9HF17O2	473.0007	6.403
M6PFDA	[13C]6C4HF19O2	519.9874	7.114
M7PFUnDA	[13C]67C4HF21O2	569.9842	7.782
M3PFBS	[13C]3CHF9O3S	302.9603	3.432
M3PFHxS	[13C]3C3HF9O3S	402.9539	5.631
M8PFOS	[13C]8HF17O3S	507.9643	7.210

Table C.2 Raw peak areas of internal standards by sample.

	Sample ID	MPFBA	M5PFPeA	M5PFHxA	M4PFHpA	M8PFOA	M9PFNA	M6PFDA	M7PFUnDA	M3PFBS	M3PFHxS	M8PFOS
		Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area	Peak Area
Calibration Standards	Cal_5_01	2,762,641	4,843,510	16,657,300	12,306,582	19,301,087	18,902,084	9,512,403	4,006,377	21,616,102	33,592,918	22,954,778
	Cal_25_01	3,310,904	5,123,545	17,486,703	12,373,303	19,069,664	16,546,783	7,093,409	2,371,650	22,484,752	34,804,455	20,654,527
	Cal_50_01	3,451,190	5,032,319	17,088,042	12,508,068	19,492,521	19,220,818	9,464,785	4,223,047	22,714,236	33,300,560	23,985,271
	Cal_100_01	3,130,851	4,654,225	15,545,499	11,198,745	17,715,070	17,492,627	8,588,106	3,934,195	19,868,586	33,592,918	20,922,027
	Cal_175_01	5,178,005	4,538,518	14,775,245	10,706,526	16,456,832	16,353,963	7,732,492	3,506,603	20,256,652	33,641,991	20,688,607
	Cal_250_01	5,015,696	4,411,648	15,195,983	10,594,831	16,255,537	17,108,988	8,187,993	3,694,815	21,562,158	33,592,918	23,401,187
Spiked Blanks	QCLO_01	3,381,365	5,112,234	17,154,222	12,243,720	17,314,037	15,376,269	9,246,420	5,902,066	20,436,273	30,451,024	23,985,271
	QCLO_02	5,509,986	2,852,398	12,855,147	8,741,845	17,203,570	18,921,641	10,110,532	4,888,776	28,054,980	34,916,242	23,882,559
	QCHI_01	3,949,301	6,066,176	19,864,353	12,212,808	17,566,721	16,546,783	9,478,944	5,335,789	24,532,260	33,422,230	24,942,831
	QCHI_02	5,563,358	2,896,016	12,812,170	8,617,599	17,346,053	19,377,235	10,946,650	5,564,842	26,571,275	33,592,918	24,657,230
Process (methods) Blanks	MB_01	3,159,564	5,376,535	18,220,829	13,346,987	20,207,362	16,546,783	8,269,369	4,507,403	22,771,418	33,970,982	23,932,945
	MB_02	5,826,911	2,743,753	11,520,387	7,928,009	16,456,832	22,359,728	19,455,812	14,683,803	25,511,061	28,493,241	28,594,992
Field Blanks	WWFB_01	4,155,593	6,483,218	22,306,131	14,629,384	19,996,735	14,162,172	6,156,525	2,957,547	27,269,544	39,763,808	23,499,643
	WWFB_02	5,022,380	2,571,861	11,303,835	7,509,338	15,366,430	16,546,783	10,241,953	5,801,753	25,699,078	33,924,352	25,100,726
	TB_02	5,379,369	2,633,767	11,691,029	7,936,658	15,928,087	17,381,477	9,773,013	5,588,983	28,115,542	35,873,881	24,742,866
Samples	INFGW_01	4,977,837	5,028,554	14,499,390	10,453,234	9,207,035	8,510,818	8,237,921	3,685,525	28,617,381	23,632,327	29,570,045
	WWDUP_01	5,459,525	5,316,126	15,526,583	10,477,087	8,791,230	7,744,334	8,203,323	3,652,267	27,269,544	23,786,942	27,783,865
	INFGW_02	5,877,639	2,600,117	10,535,289	7,077,494	15,024,764	19,897,334	18,240,172	15,627,788	27,269,544	29,838,464	28,987,148
	WWDSN001_01	4,683,728	4,923,899	15,406,063	10,662,300	10,025,211	8,516,072	8,831,362	3,939,241	32,879,448	28,006,154	27,724,225
	WWDSN001_02	4,683,728	3,222,648	14,121,873	10,394,825	20,121,320	15,816,287	10,678,677	4,532,738	27,034,943	41,260,461	25,738,680
	WWDSN003_01	2,581,030	11,846,757	12,642,980	10,011,968	15,576,616	18,791,469	12,307,195	4,911,512	31,715,317	33,592,918	33,219,826
	WWDSN003_02	3,776,749	8,366,226	13,753,341	7,766,823	16,163,685	23,698,533	12,165,541	4,312,757	28,582,113	33,592,918	43,362,087
	V770Treat_02	6,067,567	3,589,187	15,216,974	10,064,306	17,371,289	15,055,035	7,664,295	3,525,248	38,437,189	42,199,060	18,307,618
	GCUA-PS_01	3,529,228	5,464,299	18,922,064	13,041,966	18,367,844	8,966,236	4,829,936	1,282,390	44,894,474	33,592,918	11,048,014
	GCUA-PS_02	5,676,045	3,481,225	14,499,390	9,672,312	17,716,689	17,151,304	8,574,084	2,783,209	35,564,295	40,983,294	21,946,336
	EFFGCUA_01	4,683,728	3,855,012	15,114,874	12,086,996	17,407,175	14,200,892	6,808,314	3,721,338	33,279,807	42,127,268	23,296,661
	EFFGCUA_02	4,577,303	3,258,073	14,734,975	10,064,306	17,904,422	17,330,186	9,190,325	3,691,523	36,626,725	42,560,023	22,326,190
	Grand Average	4,495,230	4,677,476	15,164,840	10,541,778	16,642,734	16,241,579	9,629,243	4,912,340	27,764,248	34,152,118	24,787,265